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SURVEY STUDY OF THE EFFICIENCY AND ECONOMICS OF HYDROGEN LIQUEFACTION

UNION CARBIDE CORPORATION TONAWANDA, NY

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SURVEY STUDY OF THE EFFICIENCY

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PREFACE

The use of liquid hydrogen as a jet aircraft fuel has a number of environmental and technological advantages over conventional fuels. It is the purpose of this study to investigate that part of the system having to do with the efficiency and economics of producing liquid hydrogen using coal as the raw material. Current technology has been investigated for the best available system. Parametric studies have been made to identify where inefficiencies occur and to optimize and integrate the component parts. From this base, projections have been made to determine the minimum practicable energy and cost for producing and liquefying hydrogen in the 1985-2000 time period. The critical research and development areas requiring attention during the intervening period have been identified.

UNITS OF MEASURE

Calculations were performed for this project using the English system of units of measure. English units are also used throughout this report for presentation of results. In compliance with form PROC./P-72, the following table of factors for converting to the International System of Units (SI) is included. Appropriate conversion factors are also included with tables and graphs.

FACTORS FOR CONVERSION TO INTERNATIONAL SYSTEM OF UNITS (SI)

MULTIPLY ATM BBL BBL/TON BHP BTU BTU/HR BTU/LB BTU/LB MOL BTU/LB MOL BTU/LS MOL BTU/SCF	BY 101.325 0.15899 1.7525 x 10 ⁻⁴ 0.7457 1.05435 0.29288 2.3244 2.3244 2.3244 2.3244	TO GET KILOPASCAL METRE ³ METRE ³ /KILOGRAM KILOWATTS KILOJOULES WATTS JOULES/GRAM JOULES/MOL JOULES/MOL KILOJOULES/METRE ³ METRE ³
CU FT CFH (NTP) GPM GAL/TON HP KWH KWH/LB LB LB/CF LB/HR, CU FT LB/MM BTU LB/TON LB/YR LB MOL/HR M LB/HR MSCF/TON MSCFH MM BTU MM BTU MM BTU/BBL	0.02832 -6 7.8667 x 10-5 6.3089 x 10-6 4.1727 x 10 0.7457 3600 7.9367 0.45359 16.0185 0.12600 4.4491 4.3021 x 10 0.500 1.4383 x 10 0.12600 0.12600 0.12600 0.031217 7.8667 x 10-3 1.05435 x 10 6.6315 x 10	METRE3/SEC METRE3/SEC METRE3/SEC METRE3/KILOGRAM KILOWATTS KILOJOULE KILOJOULE/GM KILOGRAM KILOGRAMS/METRE3 GRAMS/SEC GRAMS/SEC, METRE3 KILOGRAMS/KILOJOULE GRAMS/KILOGRAM KILOGRAMS/SEC GM MOL/SEC KILOGRAMS/SEC METRE3/KILOGRAM METRE3/KILOGRAM METRE3/SEC KILOJOULES KILOJOULES/METRE3
MM BTU/HR MM CFD MM LB/YR MM SCFH	292.88 0.32778 0.014383 7.8667	KILOWATTS METRE ³ /SEC KILOGRAMS/SEC METRE ³ /SEC

MULTIPLY	BY	TO GET
PSIA	6.89476	KILOPASCAL
SCF/TON	3.1217×10^{-5}	METRE ³ /KILOGRAM
SCFH	7.8667 x 10 ⁻⁶	METRE ³ /SEC
ST/DAY	0.010500	KILOGRAMS/SEC
ST/HR	0.25120	KILOGRAMS/SEC
TON	907.185	KILOGRAMS
TON (OF REFRIGERATION)	3.5145	KILOWATTS
TPD (TONS/DAY)	0.010500	KILOGRAMS/SEC
TON/HR	0.25200	KILOGRAMS/SEC
¢/LB	2.2046	¢/kilogram
¢/MGAL	0.26417	¢/METRE ³
¢/MM BTU	9.4845×10^{-7}	¢/KILOJOULE
\$/LB	2.2046	\$/KILOGRAM
\$/MM BTU	$9.4845 \times 10_{-2}^{-7}$	\$/KILOJOULE
\$/TON	1.1023×10^{-3}	\$/KILOGRAM

°K = °C + 273.15
°K = (°F-32)/1.8 + 273.15
°API =
$$\frac{141.5}{\text{sp gr}(60^{\circ}/60^{\circ}\text{F})}$$
 - 131.5

I. INTRODUCTION

A. BACKGROUND

With the energy supply problems that we are now facing, the development of economical and socially acceptable fuels is a desirable undertaking. The use of liquid hydrogen as a jet aircraft fuel fits appropriately into this picture (24). Liquid hydrogen has many potential advantages in this role. The production of liquid hydrogen, with coal as the starting material, has been investigated in this study.

Many developments and refinements in the production of liquid hydrogen have been achieved since hydrogen was first liquefied and stored in 1898.

Tonnage plants have been built and commercially operated. An industry has developed around the production of liquid hydrogen. Dwindling supplies of natural gas, currently used as the basic raw material for hydrogen production, has intensified the investigation of other raw materials. This study has considered only one raw material - coal. It is recognized that there are other starting materials for hydrogen production and that investigations should be carried out on these other materials as well.

In the manufacture of liquid hydrogen a substantial part of the total energy is used in the liquefaction of the gaseous hydrogen and reducing the hydrogen to its lowest energy state. The attractiveness of liquid hydrogen as an aviation fuel, therefore, depends heavily upon the overall energy cost required for liquefaction. Since current processes require several times more

energy than that actually removed from the hydrogen, the possibility exists that the liquefaction efficiency can be greatly improved. It is the purpose of this study to determine the lowest practicable energy and cost for hydrogen produced from coal in the time period when hydrogen fueled aircraft might actually be in use, 1985-2000.

B. OBJECTIVES

The objectives of this study are:

- 1. Determine the minimum practicable energy and cost for liquefaction of gaseous hydrogen in the 1985-2000 time period.
- 2. Investigate the possible benefits of the integration of the coal gasification processes with the liquefaction process.
- 3. Identify and evaluate the critical research and development areas needed to achieve the objectives of Item 1 above.

C. SCOPE

To meet these objectives the study has been carried out investigating the following items:

- 1. Development of baseline technology from recently published data.
- 2. Thermodynamic and comparative analysis of the liquefaction process.
- 3. Investigate the synergistic effect on the efficiency of the liquid hydrogen production when the liquefaction process is integrated with the gas production process.
- 4. Development of energy accounting methods to properly credit by-products resulting from the combined liquefaction and gas production.

5. Projection of the potential practicable efficiencies and economics, and the research and development required to achieve them.

II. SUMMARY OF ACCOMPLISHMENTS

The theoretical work necessary to liquefy hydrogen has been determined as 14.07 kilojoules per gm (1.773 kwh per pound). The starting conditions are normal gaseous hydrogen at atmospheric pressure and 308° K. The final condition is liquid hydrogen (97% para content) at 931 kilopascals (135 psia) and 20.57°K. With this as a base condition the minimum practicable energy requirements for liquefying hydrogen was determined to be 39.06 kilojoules per gm (4.922 kwh per pound) using current technology. This gives a liquefaction cycle thermodynamic efficiency of 36.0 percent. The analysis of the inefficiencies of the practical system indicates that compression equipment accounts for more than half of this inefficiency.

The power requirement for an actual purification-liquefaction complex producing 26.25 kilograms/sec. (2500 TPD) of 97% para hydrogen as a saturated liquid at 101.325 kilopascals (1 atm) is 1,182,180 kw starting with crude normal hydrogen of 96.6% purity at 308.2°K (95°F) and pipeline pressure of 1480 kilopascals (200 psig). This is equivalent to a unit energy requirement of 45.00 kilojoules/gm (5.670 kwh/lb). With a theoretical work of liquefaction of 10.67 kilojoules/gm (1.344 kwh/lb), the thermodynamic efficiency for the total liquefaction complex is 23.7%.

Since it is possible that some of the liquid hydrogen produced could be used in the aircraft directly without intermediate storage or within a short time after being liquefied, it may be desirable to produce the liquid at a lower concentration of the para form. Significant energy saving can be obtained if the minimum conversion to para hydrogen is carried out consistent with the expected storage time. Break-even storage times have been determined to permit operation of the liquefaction unit at optimum ortho-para conversion thus yielding minimum practical energy consumption. This is an interesting concept which should be investigated in greater detail.

It appears feasible to fabricate and install liquefaction facilities as large as 2.625 kg/sec (250 tons per day) of liquid hydrogen. Ten such units operating in parallel would be used to service a major airport.

At the present time the most appropriate coal gasification process to use for hydrogen production is the Koppers-Totzek (Section IV-A). A study of this process revealed that the opportunities for integration with the lique-faction facility were limited to the coupling of energy only. Energy balances could be manipulated so as to provide for total energy requirement of both the gasifier and liquefier with no export or import power. If the Lurgi process, which operates under pressure, were used there is potential for additional integration within the purification system, which requires pressurization of the gas stream. This also applies if a Koppers-Totzek gasifier is successfully developed to operate at elevated pressures. The question of logistics plays an important role in the integration of the facilities. If all of the units are located at the same site the same air separation plant can supply the oxygen to the gasifier and the nitrogen for the nitrogen liquefier. If the units are separated, an oxygen plant and a nitrogen plant will be required.

Guidelines for determining the thermal efficiencies of processes producing potential fuels for aircraft have been suggested. Using these

guidelines the thermal efficiencies for producing the following fuels via certain processes have been determined:

Liquid Hydrogen via K-T Coal Gasification:	26.2%
Methanol via Steam Reforming of Natural Gas:	53.8%
Liquid SNG via Lurgi Coal Casification:	55.6%

Using the Discounted Cash Flow method, representative of industrial accounting and the method developed by the American Gas Association, General Accounting Committee the overall cost of producing liquid hydrogen from coal is 99 and 75 cents per kg (45 and 34 cents per pound) respectively with coal values at $\$3.32 \times 10^{-7}$ per kilojoule (35 cents per million Btu). With coal at $\$7.11 \times 10^{-7}$ per kilojoule (75 cents per million Btu), the overall cost of liquid hydrogen is \$1.23 and \$0.97 per kg (56 and 44 cents per pound) respectively. Future unit costs are expected to be more than 20% lower.

Areas for future development in both the gasification and liquefaction areas appear fruitful. The pressure gasifier would improve the efficiency and economics of the system appreciably. Additional studies look profitable on the advanced gasifiers, partial ortho-para conversion and possibly wet turbines and ejectors.

III. HYDROGEN LIQUEFACTION

A. MINIMUM THEORETICAL WORK OF HYDROGEN LIQUEFACTION

1. AVAILABILITY FUNCTION

The minimum theoretical work to liquefy hydrogen is that required to reversibly cool hydrogen from some defined initial gaseous state to another defined final state where the hydrogen exists as a liquid. It can be expressed thermodynamically in terms of the availability function which is defined as follows:

$$A_1 - A_2 = (H_1 - H_2) - T_0(S_1 - S_2)$$

The symbols H and S represent thermodynamic properties of enthalphy and entropy, respectively, while the subscripts, 1 and 2, refer to the initial and final states. $T_{\rm O}$ is the heat sink temperature at which heat is rejected to the surroundings. The change in the available energy function, A, between initial and final states represents the change in available energy for doing useful work. For the liquefaction of hydrogen, or any other cryogen, the availability function will be negative indicating a loss in available energy; that is, energy must be expended to accomplish the desired change in state.

The availability function is a thermodynamic point function. The difference in its value between two points or sets of state conditions is dependent only upon those conditions and not upon the process employed between the two points.

2. ORTHO-PARA CONVERSION

In addition to the work required to cool and liquefy hydrogen, there is another energy consuming process encountered in the liquefaction of hydrogen which arises from differences in the nuclear spin of the two nucleii which comprise the molecule. Hydrogen with molecules having nuclear spin which is symmetric is referred to as ortho hydrogen (oH $_2$) and that with molecules having nuclear spin which is asymmetric is referred to as para hydrogen (pH $_2$).

The composition of hydrogen with respect to its ortho and para modifications (1) is a function of temperature (Figure 1). This is an equilibrium phenomena; a change in temperature will cause a spontaneous change in composition until a new equilibrium composition is again attained. The equilibrium composition for liquid hydrogen at its atmospheric boiling point, 20.39°K, is 99.79% para. The para content decreases with increasing temperature until at ambient room temperature and above the equilibrium composition is only 25% para. This particular mixture, containing 25% pH₂ and 75% oH₂ is referred to as normal hydrogen (nH₂).

The need to consider para hydrogen content arises from the energy differences between the ortho and para forms. At any given temperature, the para form represents the lower energy state and in order to liquefy hydrogen and maintain it in a stable state, sufficient energy must be removed, not only to cool and liquefy the hydrogen, but also to convert it from oH $_2$ to pH $_2$. The heat of conversion from ortho to para (609 Btu/lb. mol) is a sizeable effect exceeding the heat of vaporization of nH $_2$ which amounts to 385 Btu/lb mol. The total enthalpy change in liquefying nH $_2$ and converting to 99.79% pH $_2$ is 840 Btu/lb mol.

Hydrogen conversion proceeds spontaneously although at a very slow rate. It is commercial practice, in hydrogen liquefaction, to promote the rate catalytically so that the liquid hydrogen product leaves the liquefier at near-equilibrium para content. If this is not done, the auto

conversion which occurs while the liquid hydrogen is in storage causes a severe boiloff and loss of liquid. This boiloff occurs at an initial rate of about 1% per hour (neglecting heat leak effects) and decreases with increasing conversion; the ultimate loss at infinite time approaches 69.3%

3. CONTINUOUS AND STAGEWISE CONVERSION PROCESSES

The ortho-para conversion process can be effected either in a stagewise manner or continuously. The stagewise conversion consists of alternate steps of cooling and catalytic conversion. The simplest stagewise conversion is one wherein nH₂ is cooled and liquefied and is then converted at the hydrogen liquefaction temperature. This process is not very efficient, thermodynamically, because the entire heat of conversion has to be heat pumped from the lowest temperature in the liquefaction process. The efficiency can be improved if a second stage of conversion is added at some higher temperature level, such as the temperature provided by liquid nitrogen boiling under vacuum. The larger the number of conversion stages (with intermediate cooling) the more efficient the process becomes, until, in the ultimate situation, there are an infinite number of stages and the process becomes reversible.

The continuous (3) provides for simultaneous cooling and conversion of the hydrogen stream and offers an approach to reversible conversion without the complexity of a multitude of separate cooling and conversion stages. It is accomplished in practice by passing the hydrogen feed through a bed of catalyst which is in heat exchange with a countercurrent stream of refrigerant, which may be cold hydrogen gas.

The theoretical work requirements for liquefying hydrogen by reversible conversion, by various stagewise arrangements and by

combination of reversible and stagewise processes are given in Table 1. For the 99.8% pH₂ product, the process variations are arranged in ascending order with respect to work required. The reversible process, No. 1, gives the absolute minimum work. In comparison, the single stage conversion, process No. 8, requires 35% more power. Processes No. 2 and No. 3 show that stagewise arrangements can be used at higher temperature levels (above 80°K) with very little work penalty.

Processes 9 and 10 show that up to 15% in power reduction can be achieved if a para content below 99.8% can be accepted, the savings resulting from a reduction in the heat of conversion.

4. LOW-PARA LIQUID HYDROGEN

The possible power savings in the production of low-para hydrogen prompted additional study into the acceptability of such a product. It is known that the uncatalyzed autoconversion of hydrogen proceeds slowly with a simultaneous loss of hydrogen via boiloff. If the reaction rate is sufficient-ly low and the product is consumed quickly enough after liquefaction, then boiloff losses would be low and partial conversion would be a viable process scheme.

Using the reaction rate for the ortho-para conversion as given by Scott, et al (4,5), curves showing the para hydrogen content and boil-off as a function of time for several initial values of para hydrogen concentration were derived, Figures 2 and 3. For each initial composition, a breakeven time exists for which the energy cost for conversion equals the energy cost for the vaporized hydrogen. If the hydrogen is used within the breakeven time limit, partial conversion is advantageous with respect to energy consumption. Results of this exercise, Figure 4, show a breakeven

time of 19 hours for normal hydrogen and 36 hours for 48.5% pH $_2$ (equilibrium concentration at 80° K). Breakeven times increase rapidly thereafter with para content. Prospects for making use of this concept, therefore, appear quite favorable.

Determination of breakeven times is based on either direct use of the hydrogen boiloff or recycling of it for reliquefaction. It also assumes continuous conversion for producing the partially converted liquid hydrogen product.

Figure 5 shows the theoretical work requirements for two different ways of producing partially converted hydrogen. One way is to reversibly convert hydrogen to the desired para content and the work requirement for this process is given by the lower curve. The other way is to blend normal hydrogen with the necessary amount of 99.8% para hydrogen which has been produced by reversible conversion. Although the former process is more efficient (lower curve), the blending procedure is more adaptable for producing a partially converted product over a range of compositions.

B. ACTUAL MINIMUM WORK OF HYDROGEN LIQUEFACTION

This portion of the project includes two work tasks. The first consists of a parametric study of a somewhat idealized liquefaction process for the purpose of determining the effect of varying all pertinent process variables. As part of this work task, a thermodynamic analysis was made on the liquefaction process to determine the distribution and magnitude of the various process losses. The second work task consists of the selection of a set of preferred process conditions which resulted from the parametric study and their incorporation into a realistic base case representative of the state of the art in hydrogen liquefaction

technology as of the year 1974.

1. PARAMETRIC STUDY

The parametric study was made on a somewhat idealized lique-faction process consisting of a hydrogen feed compressor, a hydrogen liquefier and a nitrogen refrigerator, Figure 6. It was assumed that pure hydrogen is delivered to the facility at atmospheric pressure and a high ambient temperature (95°F) and that the product is liquid hydrogen at 20.57°K and 135 psia, with a para content in excess of 95%. Energy requirements were based solely on process requirements; plant auxiliaries, production auxiliaries and leakage losses were not included. Plant capacity was established at 250 TPD (4,000,000 cfh) (Section III-C-5).

Evaluations were made via computer using process models constructed especially for this project. Flow diagrams for these models are presented as Figures 7 and 8.

2. HYDROGEN LIQUEFIER PROCESS

The hydrogen liquefier consists of a nitrogen precooled, expander process in which hydrogen is recycled to provide refrigeration at three temperature levels below 80°K. Two levels of refrigeration are provided by the hydrogen turbines and the third by Joule-Thomson throttling of a portion of the high pressure recycle hydrogen. At and above 80°K, refrigeration is provided by 1.) a stream of cold nitrogen gas which is used to help precool the combined feed and recycle stream and 2.) a stream of nitrogen liquid which is used for additional cooling as well as for partial ortho-para conversion of the feed stream. The hydrogen feed stream is further converted, continuously, down to the temperature level of the exhaust of the cold turbine, after which it is throttled, passed through

a catalytic converter for trimming purposes, and then subcooled in heat exchange with hydrogen boiling at low pressure.

Cold exhaust streams from the expanders are warmed in countercurrent heat exchange with cooling hydrogen streams, combined and
finally returned to the suction of the recycle compressor. Vaporized hydrogen from the final subcooler is combined with flash vapor from throttling,
warmed in heat exchange with a cooling stream and returned to suction
of the subcooling-fluid compressor which, in turn, discharges to the
suction of the recycle compressor.

3. <u>NITROGEN REFRIGERATOR PROCESS</u>

The nitrogen refrigerator, which provides cold gaseous nitrogen as well as liquid nitrogen to meet the refrigeration needs of the hydrogen liquefier, consists of an expander cycle, using dual expanders at two temperature levels plus a stage of external forecooling at 235°K. Exhaust streams from the expanders are reheated and combined into a recycle stream which is returned to the suction of the recycle compressor. The discharge from this compressor is further compressed in a pair of series-arranged boosters which are coupled to and driven by the expanders. Warm nitrogen gas is returned from the hydrogen liquefier, recompressed as necessary, and mixed with the nitrogen recycle stream. Cold nitrogen product gas is removed as a portion of the cold expander discharge. The remainder of the cold expander discharge is used for final cooling and liquefaction of the product nitrogen.

4. PROCESS BALANCES

For the parametric study, a series of process balances were made on the hydrogen liquefier for the purpose of observing the influence

of a variety of process parameters on the unit power required for liquefaction of the hydrogen. Only the hydrogen liquefier was subjected to the study with the one exception where all process compressors were taken into account in determining the effect of compressor efficiency. The nitrogen refrigerator was excluded on the basis that its performance is sufficiently well known that a parametric study would be unwarranted. Shaft work from the expanders is recovered and credited against the total compressor work so that net work requirements are reported. Table 2 lists all parameters included in the study and cites figure number references for calculated results. Table 5 lists values of base parameters which were always maintained constant except for the parameter being varied.

5. RESULTS OF PARAMETRIC STUDY

The results of the parametric study are presented in Figures 9-18, inclusive. Comments concerning each of the figures follow:

FIGURE 9. HYDROGEN FEED PRESSURE

Increasing the feed pressure increases the expander work output and causes a reduction in the recycle flow. Although the recycle compressor ratio has increased, the flow is dominant up to a pressure of 600 psia where a minimum exists in unit work requirement.

FIGURE 10. RECYCLE BACK PRESSURE

Increasing the back pressure decreases the expander work output and increases the recycle flow. However, in this case, the compression ratio is dominated and unit work requirement decreases with increasing back pressure up to 52 psia. Higher back pressures produce a two-phase exhaust on the cold expander unless the constraint on the constancy of the exhaust temperature is removed. Higher back pressures reduce pressure losses in

the return recycle stream when passing through heat exchangers. This effect is accounted for.

FIGURE 11. MINIMUM REFRIGERATION LEVEL

This refers to the exhaust temperature from the cold level expander, E-2. Raising this temperature level diverts a larger fraction of the low temperature refrigeration load from the expander to the less-efficient Joule-Thomson refrigeration and increases the unit work requirement. Minimum work, within the range considered, occurs at an exhaust temperature of 26°K. This is approximately 0.7°K from the saturation temperature at the exhaust pressure and further lowering of the temperature would produce a two-phase exhaust stream.

FIGURE 12. EXPANDER EFFICIENCY

This refers to the isentropic efficiency of the two hydrogen expanders. Efficiency was varied from 77% to 85% and produced a reduction in work requirement of 5.4%. The efficiency range covered represents, for hydrogen service, what may be considered mediocre performance at the low end and very good performance at the other. Typical present day efficiencies of about 80% can be expected. A base efficiency of 79% was used for the parametric study.

FIGURE 13. COMPRESSOR EFFICIENCY

This parameter refers to the adiabatic efficiency of all process compressors, which includes:

1.	H_2	recycle compressor	•••	80%
2.	н ₂	subcool fluid compressor	-	80%
3.	н ₂	feed compressor	-	80%
4.	N ₂	recycle compressor	-	80%
5.	N ₂	makeup compressor	-	75%
6.	N,	booster compressors	_	65%

Not all compressors were assigned the same efficiency; some attempt was made toward realism. The preceding percentage values are the adiabatic efficiencies assigned for each compressor. The performance curve, Figure 13, presents results as a function of departure from these assigned values. That is, a two-percentage point increase signifies a like increase for all compressors. A ten-percentage point increase in efficiency produces a 12.6% reduction in work requirement. The weighted average for the above assigned efficiencies is 79%.

FIGURE 14. PARA CONTENT

This parameter is based on continuous conversion of the feed stream to the desired composition followed by further cooling, liquefaction and subcooling. The trim converter, C-5, is, of course, omitted. The actual power requirements are nearly in constant proportion to the theoretical power requirement as presented in Figure 14. Accounting for losses in flashing the product hydrogen to atmospheric pressure, the thermodynamic efficiency (ratio of theoretical to actual work) for partial conversion varies as shown in Table 6.

FIGURE 15. WARM END TEMPERATURE APPROACH

This refers to the temperature differences between process streams 4 and 46, 81 for heat exchanger X-1 and process streams 2 and 57, 95 for heat exchanger X-8. Increasing the temperature approach reduces the heat exchanger surface requirement but increases the process refrigeration requirement, and, hence, the unit work. An 8°K increase produces a 3.6% work increase but decreases the heat transfer surface required by 41%. This a matter of economic analysis in optimizing the heat exchanger.

FIGURE 16. WARM END TEMPERATURE APPROACH

This parameter refers to the temperature difference between streams 25 and 36 of heat exchanger X-3 and streams 12 and 43 of continuous catalytic converter XC-3, the difference between this and the preceding parameter is that now the additional refrigeration load imposed on the system must be supplied by the hydrogen turbines rather than by the less costly nitrogen refrigeration. An increase of 4.7°K in this parameter produces a 5.7% work increase and a 40% decrease in the heat exchanger surface requirements. The size of heat exchangers X-1, X-3, and X-8 are affected by this parameter as well as heat exchanger X-3 and converter XC-3.

FIGURE 17. COLD END TEMPERATURE APPROACH

This parameter applies to nitrogen-forecooling heat exchanger X-2 and catalytic converter XC-2. It is the temperature difference between streams 88 and 21 and between streams 86 and 11. Figure 17 reveals that both work and heat transfer surface are relatively insensitive to variations in this parameter.

FIGURE 18. REFRIGERATION ARRANGEMENT

In this portion of the study, a different method for providing refrigeration at and above the $80^{\circ} K$ level was investigated. It is, therefore, a process rather than a parmetric variation.

The process variation consists of substituting a hydrogen turbine to provide the refrigeration normally supplied by liquid nitrogen and by cold nitrogen gas. A stream of hydrogen is bled from the feed stream after a certain amount of precooling and passed through the turbine. The turbine exhaust stream is then used for cooling, via its sensible heat

content, in heat exchangers X-2, X-1 and X-8 as well as converter XC-2. In the process, the additional hydrogen required for refrigeration becomes part of the recycle stream and is recompressed in the recycle compressor. Table 7 compares process requirements for the expander process with requirements when using nitrogen for refrigeration. The large increase in recycle flow required to maintain a refrigeration balance results in a 37.5% increase in power.

6. BASE CASE SELECTION

Based on the results of the parametric study, a set of process conditions was selected to represent the base case. Table 3 presents a tabulation of all stream data and process conditions for the hydrogen liquefier while Table 4 presents stream data and process conditions for the nitrogen refrigerator required to sustain the chosen hydrogen liquefier. The net power required for producing 250 TPD of liquid hydrogen for the same set of assumptions used in the parametric study amounts to 137,540 BHP which is equivalent to a unit work requirement of 4.92 KWH/LB, Table 8. Emphasis must be made that this constitutes a power requirement for a somewhat idealized set of process assumptions. Subsequent work takes into consideration a more realistic process case (Section III-C-3), and a real-life power requirement somewhat greater than the 4.92 value reported here can be expected.

The nitrogen refrigerator additions listed in Table 8 refer to:

1) Nitrogen refrigerator power required to produce the cold nitrogen gas (Figure 7, Stream 92) which returns from the hydrogen purifier and not originally charged to the refrigerator unit.

2) The additional available energy required in the liquid nitrogen stream resulting from a mismatch in specified process conditions at the nitrogen refrigerator (Figure 8 and Table 4, Stream 18) and the hydrogen liquefier (Figure 7 and Table 3, Stream 83).

7. THERMODYNAMIC PROCESS ANALYSIS

A thermodynamic analysis was conducted on the idealized base case for the purpose of determining the distribution and magnitude of the process irreversibilities, or losses. Identification of the major sources of process losses can spotlight process areas and items of equipment where effort can be expended most effectively in improving process efficiency. Process factors which contribute to irreversible work losses include finite temperature differences in heat exchangers, departures from isentropic compression and expansion in compressors and turbines related to machinery efficiency, pressure reductions across throttling valves, mixing of unlike streams, and heat leak.

Results of the analysis are presented in Table 9 for the hydrogen liquefier, in Table 10 for the nitrogen refrigerator and in Table 11 for a consolidated summary of total losses, categorized by process and by equipment type. The latter table shows that the hydrogen liquefier is the main process contributor to process losses (at over 66%) and that compressors are the major equipment contributor (at nearly 53%). It is shown in Tables 9 and 11 that the hydrogen recycle compressor is the largest individual contributor, with a process loss amounting to over 28% of the total process loss. The nitrogen recycle compressor, P-3, is the second largest individual contributor. Any development leading to improvement in the compression

efficiency of these two compressors would be effective in improving overall process efficiency.

Other areas where significant improvement may be possible are the hydrogen turbines and heat exchanger X-3 of the hydrogen liquefier. This heat exchanger has an inordinately large process loss compared with the rest of the heat exchangers and suggests that the temperature approaches selected may not be optimum. The resulting thermodynamic efficiency for the complex comprising the hydrogen liquefier, the nitrogen refrigerator and the feed compressor is 36.0%.

The total actual work of 4.9254 kwh/lb as listed in Table 11 is in substantial agreement with the value of 4.9217 kwh/lb as listed in Table 8 and constitutes an overall available energy balance check. The discrepancy of 0.08% can probably be attributed to rounding errors.

The value for theoretical work as listed in Table 11 and amounting to 1.7728 kwh/lb will not check the value of 1.799 kwh/lb for reversible theoretical work as listed in Table 1 because feed and product process conditions are not the same in each case.

C. ACTUAL BASE CASE HYDROGEN LIQUEFACTION COMPLEX -

1. <u>1974 BASIS</u>

The idealized base case previously developed and described formed the basis for the actual base case process. The actual case is a realistic representation of the total liquefaction complex, based on current technology, which must be provided in order to meet the fuel needs of an aircraft servicing facility. It assumes that the liquefaction complex is separate and apart from the coal gasification portion of the process except as it receives feedstock and power therefrom. No attempt has been made to geographically define

the relationahip between the mine, the gasification plant and the liquefaction plant because of the nature and magnitude of the accompanying logistics problems. The actual case merely assumes that crude hydrogen feedstock is received under pressure from a pipe at battery limits. Energy, in the form of electrical power generated at the gasification plant, is also received at battery limits. Again, no study has been made of the best way to convert, transport and provide the necessary energy to drive the compression machinery and operate other equipment at the liquefaction site. All prime movers are assumed to be electric motors.

The actual base case also takes into account realistic process allowances such as energy requirements for cryogenic hydrogen purification, leakage from machinery and cold box equipment, efficiencies of electric motors, gear losses where applicable, production auxiliaries such as cooling tower and instrument air requirements, and plant auxiliaries such as lighting and heating. Table 12 lists the assumptions which form the basis of the actual base case.

2. HYDROGEN PURIFICATION

The actual base case includes a final hydrogen purification step which was not part of the idealized base case. This needed for the purpose of purifying hydrogen to liquefaction-grade quality to permit cooling to the hydrogen liquefaction temperature without plugging of equipment from freezeout. Impurity levels in the order of one ppm total content of non-hydrogen species is typical for this purpose.

Two commercialized technologies exist for purification of hydrogen to liquefaction grade. A cryogenic absorption purification process (6) has been chosen in the present study. The other is a thermally-regenerated

cryogenic adsorption process (7) which is described and compared with the adsorption process elsewhere in this report (Section III-C-6). Both absorption and adsorption processes have been used commercially, each having a cumulative production total of nearly 100 TPD of liquid hydrogen in support of the Apollo Program.

The absorption process consists of two cryogenic absorption stages in series in which liquefied light hydrocarbons are used as absorption fluids. In the first absorption stage, light components such as nitrogen, carbon monoxide and argon (if any) are removed by scrubbing with subcooled liquid methane. The overhead hydrogen from the absorber will contain methane in amount equal to the equilibrium composition, usually about 1%. The purpose of the second absorption stage is to remove this methane, and, for this, deeply subcooled liquid propane is used as the scrubbing agent. At a temperature of 90°K, the vapor pressure of propane is so low that overhead contamination is negligible. The only additional processing is a final adsorption step in which a small bed of adsorbent is used to remove remaining trace quantities of impurity and to provide guarding action against upset. Absorbent streams are purified, by distillation in the case of the methane, and by stripping with a small portion of the product hydrogen stream in the case of the propane. Purified liquids are recycled to their respective absorbers.

Because the absorption and purification operations take place at different temperature levels, a heat pumping system is included as an integrated part of the purifier. Nitrogen is recycled as the working fluid, necessitating a recycle compressor and a consumption of energy. Refrigeration requirements to sustain the purifier are provided via liquid nitrogen from the nitrogen refrigerator.

3. UTILITY SUMMARY

A summary of utilities required for a 2500 TPD hydrogen liquefaction complex based on the block flow diagram, Figure 19, is given in Table 13. The complex consists of 10 liquefaction modules, in parallel, each module producing 250 TPD.

Power requirements are presented in two columns. The first column shows the brake horsepower requirement for the particular item of machinery listed. The second column lists electrical power requirement, in kilowatts. In the case of compressors, this a straightforward power conversion, allowing for electric motor efficiency and gear losses, if any. For other pieces of equipment, additional consumption of electrical energy may be involved, such as for electrical heaters.

Total net electrical power consumption amounts to 1,182, 180 KW which is equivalent to a unit consumption of 5.670 kwh/lb liquid hydrogen product. The theoretical minimum work of liquefaction for the 200 psig feed in stream is 1.344 kwh/lb so that the thermodynamic efficiency for the actual base case amounts to 23.7%. This compares with the 36% efficiency calculated for the idealized base case, Table 11.

The electrical energy is provided by the power section at the coal gasification site.

4. MANPOWER REQUIREMENTS

Total manpower requirements for operating and maintaining the 2500 TPD liquefaction complex amount to 169 persons. This breaks down into four operating shifts of 26 men plus four maintenance shifts of 10 men. Each operating shift is provided with a cryogenic operator plus a compressor attendant for each plant module, 5 assistant operators and a chief

operator. Each shift will also require 1 foreman. In addition, a plant superintendent, two assistants, two plant engineers, two instrument men, one analyst for quality assurance, a foreman supervisor and twelve office personnel will be required.

The preceding manpower provides only for plant operating and maintenance requirements. Distribution and aircraft servicing personnel would be additional.

5. PIANT CAPACITY AND EQUIPMENT LIMITATIONS

Several key items of equipment were examined for the purpose of relating liquefier module sizes to size limitations of commercially available equipment. Cost information was also applied to determine whether the usual cost-capacity advantage for large capacity plants was significant for the module capacity selected.

The largest liquid hydrogen plant which has, heretofore, been commercially built and operated had a capacity of 60 tons per day, but this was not strictly a single train plant. The recycle compressor, a major equipment item, consisted of a pair of reciprocal compressors, in parallel, each compressor being near the limit of commercial availability with regard to size. Also, many of the heat exchangers within the cold boxes were multiple units, installed in parallel.

Accepting a considerable amount of paralleling of equipment, it should be possible to build a 250 TPD plant having a single cold box each for the purifier, the liquefier and the nitrogen refrigerator. The

hydrogen recycle compressor and subcooling recompressor would be combined into 6 parallel reciprocating compressors having a total power requirement of 83,699 bhp for the module. The cold box casing would have the approximate dimensions of 75 ft. diameter x 60 ft. high for the liquefier, 65 ft. diameter x 60 ft. high for the purifier and 30 ft. diameter x 35 ft. high for the nitrogen refrigerator.

The purifier distillation columns are within size limitations for shop fabrication and shipment. For any significant increase in capacity, they would have to be field fabricated where a certain amount of control over fabrication procedures and quality must be relinquished.

Comparative cost estimates for capital investment for both 250 TPD and 500 TPD modules show the exponent on capacity-cost equation,

 $cost = a(capacity)^n$,

to be 0.95 over this capacity range, indicating that there is no investment advantage in building larger modules. The exponent for paralleling of ten 250 TPD modules is 0.963.

Plants are therefore assumed to consist of parallel production modules of 250 TPD capacity each. The 2500 TPD liquefaction complex consists of 10 such modules.

6. ABSORPTION VS ADSORPTION PURIFICATION

The crude hydrogen feedstock as obtained from the coal gasification unit is only partly purified; it has a 96.6% purity with the remainder

consisting of carbon monoxide, nitrogen, argon, methane, carbon dioxide, and water vapor. Before it can be liquefied, the feedstock must be subjected to a final stage of purification from which liquefaction grade hydrogen emerges having a total impurity content of 1 ppm. This final purification is accomplished via cryogenic processing.

A comparison was made between a cryogenic absorption purifier and a cryogenic adsorption purifier. The difference is that with the absorption unit, impurities in the hydrogen feedstock are removed in a continuous process by physical solution in a suitable absorbing liquid, while in the adsorption process the impurities are removed in a batchwise process by physical adsorption on the surface of a suitable adsorbing solid. The absorption process is the one chosen for the actual base case study and is described in another section of this report (Section III-C-2).

The adsorption process consists of passing the impure hydrogen feedstock through an adsorber consisting of a bed of silica gel under 600 psia pressure and at 100°K. The silica gel removes the impurities by physical adsorption thereon yielding a purified hydrogen of liquefaction grade. The adsorbers are sized for an 8-hour on-stream period, after which they are removed from service and replaced with an alternate set of freshly reactivated adsorbers.

The reactivation process consists of heating the adsorber beds to a temperature level of 100°F. At elevated temperatures, impurity loadings on the silica gel are greatly reduced and the impurities are given off, aided

by a purging operation. The specific reactivation procedure requires the recirculation of a gas stream, by means of a recirculating blower, through the adsorption vessels, through an economizer and return to the blower. The economizer consists of a regenerative heat storage vessel which is used to conserve refrigeration. As the cold gases emerge from the adsorbers they are used to cool down the storage mass contained within the economizer. Reversal of the gas stream returns refrigeration from the economizer to the adsorber bed for recooling.

As impurities are described, pressure, which would tend to build in the recirculating loop, is relieved by means of relief valves. When the entire adsorber is at the final temperature level, the circuit is depressurized and a stream of pure product hydrogen is used to purge the system. A reactivation heater is included in the circuit to assist in obtaining final reactivation temperature. During the latter operations, the economizer would be by-passed, while still storing refrigeration.

The next reactivation step is to place the adsorbers in an on-stream ready condition. The adsorbers and recirculating system are pressurized with pure product hydrogen to operating pressure and the recirculating compressor circulator gas in the reverse direction from the compressor to the economizer and thence through a liquid nitrogen cooler to the adsorbers. By use of the economizers, the only nitrogen required is for makeup of refrigeration losses.

Results of the comparison between the absorption and adsorption purifier are given in Table 14. Although the estimate investment for the

adsorption purifer is one million dollars greater, operating power requirements are less by about 550 kw. Despite the use of the economizer, a substantial amount of liquid nitrogen is still required for adsorber cooldown. The difference in refrigeration between the two purifiers is greater than indicated by liquid nitrogen consumption inasmuch as the absorption purifier uses only the latent heat refrigeration and returns the cold vapor to the hydrogen liquefier whereas the adsorption purifier uses both latent and sensible heat refrigeration. Hydrogen losses via leakage, purge, blowdown, venting, stripping, etc. are comparable for both processes as is cooling water usage. The overall differences between the two types of purifiers are not sufficient to produce a major impact on the total liquefaction complex.

7. PROCESS LEAKAGE LOSSES

Loss of gaseous streams because of leakage has been treated in detail for the hydrogen liquefaction complex. Table 27 lists the losses by source and by amount. These are realistic values based on experience.

No allowance has been made for leakage losses in the gasification complex. Source and amount of leakage would depend strongly on the type and specific design of equipment which has not been specified. This report contains sufficient detail and information, however, to permit the reader to include his own values for leakage allowance should he so desire.

Leakage losses can also be expected for the pipelining of crude hydrogen between the gasification and liquefaction complexes. These have

not been accounted for in this study because the geographical relationship between the gasification and liquefaction sites has not been defined. Once this relationship is known, typical pipeline gaseous losses can be anticipated.

IV. COAL GASIFICATION

A. BASE CASE

There are several coal gasification processes in commercial use today which could be used to produce hydrogen from coal. In general, such a system would consist of a gasification section followed by any gas clean-up, compression, shift reactions or reforming necessary to produce a gaseous hydrogen stream suitable for feeding to a hydrogen liquefaction system.

The base case of this study consists of three major systems:

- 1. Feedstock gasifiers consisting of a Kopper-Totzek gasification process and the gas clean-up and conversion processes necessary to produce a stream of gaseous hydrogen.
- 2. Power plant gasifiers consisting of a Koppers-Totzek gasification process and gas clean-up processes necessary to produce a clean, low Btu fuel gas to provide the power for the feedstock gasifier and for the hydrogen liquefaction.
- 3. A hydrogen liquefaction system consisting of a purifier and a liquefier.

For this study the Koppers-Totzek process (8,15) was chosen as the standard coal gasification process to be used in conjunction with a hydrogen liquefaction system since it is a commercially available gasification process which is well-suited to hydrogen production. All types of coals may be used without pre-treatment, and it is a relatively clean and pollution-free process which does not produce any tar, oil, or phenols. The product gas is high in

hydrogen and carbon monoxide content, and the CO can be shifted to produce even more hydrogen. Negligible methane is produced in the gasifiers so that no reforming is required. The major energy requirements of the system are in producing the required amounts of oxygen for the gasifiers, steam for the CO shift conversion and gas purifications, and in compressing the raw gas stream.

Since the liquefaction section itself requires over a thousand megawatts of power, the base case includes a power generating facility so that the overall system will require no power other than what is derived from the coal used by the plant - i.e. the overall complex will be self-sufficient. (The presence of sulfur in coal complicates direct power generation.) To simplify the base case it is assumed that the power generating section will also use K-T gasifiers.

The base case as shown in Figures 20 and 21 is a starting point only. It is not claimed that this case represents the optimum operating conditions since there are many possibilities for improvement. However, the overall system is composed entirely of processes in commercial use today.

Block diagrams of the base case sections for using K-T gasifiers to produce hydrogen and power are shown in Figures 20 and 21. The initial processes - coal handling, drying, and preparation, gasification, heat exchange, and compression and cooling - of both sections are similar. The coal used for the base case is a typical Eastern coal containing 3.5 wt. % of sulfur.

Coal is dried and then pulverized to about 70% through 200 mesh. Pulverized coal entrained in oxygen and low pressure steam is fed through burner nozzles into the gasifier itself. Reaction temperature at the burner discharge is 3300-3500°F, and the operating pressure is slightly above atmospheric. Fixed carbon and volatile matter are gasified to produce a raw gas composed of mostly CO and H₂ while the coal ash is converted into a molten slag. About 50 percent of the slag drops into a water quench tank. Low pressure steam for the gasifier reaction is produced in the gasifier jacket from the heat passing through the refractory lining.

Gas leaving the gasifier is quenched with water to solidify the entrained slag and is passed through a waste heat boiler where high pressure steam is produced. Then the gas is scrubbed to remove entrained solids and compressed. The product gas from the power plant gasifiers need only be compressed enough to allow for system pressure drops and the gas turbine operational pressure of approximately 150 psia. Since the gas product of the feedstock gasifiers will eventually be compressed to 600 psia in the liquefier section, part of the compression is performed at this point to aid in the acid-gas removal and shift-conversion steps.

Since the base case assumes that a 3.5 weight % sulfur coal is being used, the gas at this point in the processing will contain over 1% sulfur compounds. The fuel gas stream must be purified enough so that a sulfur emission standard of 1.2 pounds of sulfur per million Btu's can be met when

that the low temperature water-gas shift catalyst will not be poisoned. A standard process which may be used for these required sulfur removals is the Rectisol process (16,17) - a physical absorption process using cold (-60°F) methanol as the solvent. Rectisol takes advantage of the good selectivity of H_2S over CO_2 in methanol and high absorption capacity at low temperatures and elevated pressures. Regeneration of solvent is simple. Most of the CO_2 absorbed in the methanol can be released by simple flashing and the rest of the solvent regeneration can be accomplished by stripping or distillation. After the bulk of the sulfur compounds are removed by Rectisol, the fuel gas is ready for use in the power generating equipment while a guard trap, if necessary, may be used to complete the removal of the sulfur compounds from the gas which will be used as a feedstock.

The water-gas shift reaction (CO + $\rm H_2O \rightleftharpoons \rm CO_2 + \rm H_2$) is widely used for the manufacture of hydrogen (18, 19). After sulfur removal, the product gas contains over 50% CO, most of which can be catalytically shifted to hydrogen by the water-gas shift reaction. For the base case, the conversion will be carried out in two stages. The first stage will use a relatively inexpensive high temperature (600-900°F) catalyst while the second stage will use a more expensive low temperature (350-500°F) catalyst to complete the required conversion since the equilibrium constant for the reaction is much larger at the lower temperature. The product gas from the water-gas shift reactor will be approximately a 60-40 mixture of hydrogen and CO₂ with less than 1% CO.

This large concentration of ${\rm CO}_2$ must be separated from the hydrogen before sending the gas through the purification system associated with the

liquefaction section. A commercial process (20, 21) favored by the high CO_2 concentration is the hot potassium carbonate absorption process, which has the advantages of a low investment and low stream consumption. In the base case, hot carbonate absorption would be used to reduce CO_2 concentration of the product gas from 38% to 0.25% to produce a hydrogen stream of 95% purity.

Since logistics and site location are beyond the scope of this study, the base case has been considered to be the three separate sections described previously with no allowances made for possible logistical problems involved in transferring energy or material from one section to the other. Approximately 22% of the fuel gas produced by the power plant section will be used as a clean, low-Btu fuel to make the steam for the hydrogen production section and to dry the coal; 23% will be burned in Frame 7 gas turbines to produce power for the gas compression step and part of the power for the oxygen plants. The remainder will be burned in Frame 7 gas turbines and converted to electricity for the liquefaction section and for the acid-gas removal steps, coal handling and preparation, and plant auxiliaries. Most (96%) of the power for the oxygen plants and for part of the gas compression will be taken from steam turbines using the high pressure steam produced by the waste heat boilers following the gasifiers.

The base case presented above is believed to be the most straightforward commercial means of producing liquid hydrogen from sulfur bearing
coal in a self-sufficient manner. Although no optimization has been
attempted, it, nevertheless, is a representative case which cannot be
improved greatly without advanced coal gasification, gas purification,
and hydrogen liquefaction technology. Thus, the economics and performance
given in latter sections are representative of the state of the art.

- B. OTHER COMMERCIAL GASIFIERS As a point of reference, the base case with the Koppers-Totzek gasifier is represented in Figure 22. The raw gas composition is most favorable for hydrogen production because only water gas shift and gas purification is required. The disadvantages as noted in the previous section are that the product is at low pressure and that more oxygen is required than in most advanced gasifier processes. The greater oxygen quantity reflects itself in higher oxygen plant investment but not in operating cost because the K-T gasifier inefficiencies are being utilized to generate the energy for air separation. With this base case as background, two other commercial gasifiers are discussed below.
- 1. The Lurgi gasifier is depicted in Figure 23. The main advantage of the Lurgi gasifier is that it is a pressure gasifier giving a raw gas at 20 to 25 atmospheres. This advantage results in the elimination of the gasifier product gas compressor and equally important the opportunity to water gas shift the

carbon monoxide to hydrogen and carbon dioxide without cooling the gasifier product gas for compression. Thus, significant steam requirements can be saved. In addition to the usual mechanical problems of feeding coal and removing ash from high pressure reactors, the main disadvantages are that 19% of the product Btu's are in the form of tar, tar oil, naphtha, and crude phenol and that the raw gas, as tabulated in Figure 23, contains a significant amount of methane. The crude liquids might be burned with some care because of potential health considerations, but the methane contains too much hydrogen to be used for fuel. The expectation is that the methane would be reformed to hydrogen after low temperature separation or be sold to a gas utility as a by-product depending upon the logistics of the gasification location. A more detailed evaluation of the Lurgi pressure gasifier for hydrogen production is desired, but on the surface it seems that the pressure advantage might be counterbalanced by the more difficult gas purification and utilization of the by-products.

2. The Winklergasifier, depicted in Figure 24, is an atmospheric gasifier which operates on the fluidized bed principle. It was first commercialized at Leuna in 1926. Since then 36 producers at 16 installations have been designed, engineered, constructed and commissioned all by Bamag Verfahrenstechnik GmbH, a German affiliate of Davy-Power Gas. Some tars and tar oils are also produced in addition to the raw gas listed in Figure 24. While improvements and pressurized operation might be successful

in the future, as this process stands today it has the disadvantages of both Koppers-Totzek and Lurgi without their advantages.

Although it is desirable to better assess the Lurgi gasifier, it is believed that the Koppers-Totzek gasifier chosen for the base case is the most attractive commercial gasifier available for hydrogen production from coal.

- C. <u>ADVANCED COAL GASIFICATION PROCESSES</u> A short discussion of advanced coal gasifiers will be presented to suggest potential studies for hydrogen production improvement. Most advanced coal gasifiers are high pressure and are developed for the production of synthetic natural gas. Work on advanced versions of pressure Koppers-Totzek, Winkler, Shell, and Texico gasifiers are more adaptable to hydrogen production except for perhaps the CO₂-Acceptor and Union Carbide Agglomerated-Ash Process.
- 1. Hygas, pilot planted by IGT, is one of the more advanced SNG processes. Figure 25 illustrates the three versions of hydrogen production for coal hydrogenation in the main three-stage gasifier. As noted from the typical raw gas compositions, the Hygas process is geared to produce SNG and not carbon monoxide and hydrogen; but, developments in learning how to feed coal into the high pressure reactors are useful for all coal gasification processes producing hydrogen. In order to gain a more complete picture, the concept of coal hydrogenation to produce char and hydrocarbon rich raw gas should be studied for hydrogen production wherein char is used for fuel and hydrogen is produced by reforming. This necessitates hydrogen

gasifier recycle; but, carbon dioxide rejection is decreased.

- 2. Synthane is an advanced partial oxidation process being pilot planted by the Bureau of Mines in Bruceton. This process is depicted in Figure 26. To some degree, Synthane is like piecing Hygas and an oxygen gasifier together. The similarity can be observed in the raw gas compositions tabulated in Figures 25 & 26. The hydrocarbon rich raw gas would again be reformed for hydrogen production while a portion of the char would be utilized in a power plant as depicted in Figure 26.
- 3. CO₂ Acceptor process is another advanced process. The novelty of this process as shown in Figure 27 is that heat for the carbon-steam reaction is provided by reacting the CO₂ formed with calcined dolomite. Removal of CO₂ enhances the water gas shift reaction. Heat for regenerating spent dolomite is supplied by burning char with air in the Dolomite Regenerator. Because of the characteristics of ash, dolomite, and coal reactivity, this process has only been suggested for lignite. However, the general concept of a CO₂-Acceptor for driving the water gas shift is most interesting. The Linde Division of Union Carbide has examined the phenomena in hydrogen production from methane rich streams in which hydrocarbon reforming and CO₂ removal are combined wherein the heat of reaction of CO₂ with the acceptor in this case furnishes the heat for hydrocarbon reforming. There is uniqueness to the CO₂-Acceptor concept for hydrogen production and should be investigated coupled with one or more coal gasification techniques.

- 4. <u>Bi-Gas</u> is a process being developed by the Bituminous Coal Research, Inc. This is a two stage partial oxidation process similar to Synthane, but, with new equipment concepts and operating at higher temperatures to minimize tar liquids. Raw gas composition listed in Figure 28 also suggests methane reforming requirements. A 120-ton/day pilot plant to produce 2.4 million SCFD is under construction at Homer City, Pennsylvania. Advantage for hydrogen production is the high gasifier pressure just as in the other advanced gasifiers.
- 5. <u>Hydrane</u> is a process being developed by the Bureau of Mines based upon coal hydrogenation as depicted in Figure 29. Raw gas composition is the highest in methane of all the advanced SNG processes and would certainly require methane reforming for hydrogen production.
- 6. <u>Union Carbide's Agglomerated-Ash Process</u> might be an interesting process for hydrogen production because of the low methane composition in the raw gas at conditions of 100-150 psig and 1900°F given in Figure 30
- 7. <u>Kellogg Molten-Salt Process</u> is illustrated in Figure 31 along with typical raw gas compositions. The main novelty is the molten salt which transfers the heat for the steam-carbon reaction from the exothermic carbon-oxygen reaction.
- 8. Atgas Process is shown in Figure 32. Rather than a molten salt, as applied in the Kellogg process, molten iron is utilized. Conditions are such that more methane appears in the raw gas.

All the advanced processes have in common the fact that coal gasification is done at elevated pressures either by way of coal partial oxidation or coal hydrogenation.

D. <u>COAL LIQUEFACTION</u> - Although it is beyond the scope of this program to discuss logistics and other fuels, for completeness sake and presentation of suggested work, a short discussion of coal liquefaction will be given.

Production of liquids from coal was practiced in Europe during World War II. Processes such as Fischer-Tropsch Synthesis (Figure 33) and hydrogenation processes similar to H-Coal (Figure 34) and Synthoil (Figure 35, were used by the Germans. Pyrolysis processes such as CO-ED (Figure 36) and Consol Synthetic Fuel (Figure 37) are extensions of coke oven and coal pyrolysis technology. The liquefaction process which might have the greatest impact on coal hydrogen production and logistics might be the Solvent Refined Coal (SRC) process given in Figure 38. This process removes sulfur and ash from run-of-the-mine coal possibly near the mine to give approximately 15,800 Btu/lb coal which can be liquefied by heating. The fact that SRC can be reliquefied by heating would offer excellent opportunity for very simple gasifier feed system design for high pressures. Being essentially ash-free reduces the gasification to the problem of residual oil gasification. With sulfur removed, the power generation portion of the facility now can be conventional or an advanced power cycle with gas turbines coupled with steam turbines. The SRC process should be studied for possible application for 1985 and beyond.

V. THERMAL EFFICIENCIES

A. <u>ACCOUNTING RULES</u>

The efficiency of a fuel gas process can be described in terms of the percentage of the heating value in the input fuel which appears as heating value in the product stream. This is referred to as the thermal efficiency. If there is only one source of input energy and only one stream of output energy, the definition of thermal efficiency is straightforward. If there are more than one source and kind of input energy and several by-product streams which have heating value, a set of accounting rules must be established in order for the term "thermal efficiency" to be meaningful. The set of accounting rules for determining the thermal efficiency of the actual base case liquefier (1974) is as follows:

- 1. Thermal efficiencies are based on gross heating values of fuels.
- 2. Gross heating values are 61,100 Btu/lb for hydrogen and 12,500 Btu/lb for coal. (lower heating values are 51,623 Btu/lb and 12,000 Btu/lb, respectively.
- Credit is taken for all by-product combustible streams, which can be burned in a practical manner, by recycling to the gasifier.
- By-product streams which cannot be burned in a practical manner, such as sulfur and ammonia, are not credited.
- 5. No allowance is made for possible energy or material losses between the major process units (i.e. feedstock generation, power generation, hydrogen liquefier) on the basis that the logistics involved have not been defined within the scope of this study (Section VI-A).

- 6. Heat rejected via cooling water has no usable value and is not credited.
- 7. Electrical energy for both gasification and liquefaction complexes is generated in the power gasifier section. No additional outside source of power is required.
- 8. Thermal efficiency of hydrogen liquefier is based on heating value of feedstock plus electrical energy as energy input, and heating values of product hydrogen and tail gas as the only output.
- 9. The complete hydrogen generation and liquefaction complex is entirely self sufficient. All power for processing as well as plant auxiliaries is generated within the complex.

B. POWER USAGE BREAKDOWN

1. HYDROGEN LIQUEFACTION

Thermal efficiency for the production of liquid hydrogen from coal is presented in Table 15. The presentation shows input and output energy streams for each of four processing sections of the combined complexes. Although a two-way division for the total plant is used throughout most of this report, a four-way division is used here to more clearly draw attention to where the major energy losses occur. The four sections receiving attention are:

- 1. The feedstock gasifier section
- 2. The power gasifier section
- 3. The hydrogen liquefaction complex
- 4. The energy conversion section

The following tabulation presents a summary of the thermal

efficiencies for each of the four sections as well as the overall thermal efficiency. Although heating values of fuels are usually given in terms of the higher heating value, the tabulation also presents the corresponding thermal efficiency based on lower heating values. See Section V-B-3 for a listing of heating values

	Thermal Efficiency - %	
Basis	HHV	LHV
Feedstock Gasifier	58.6	51.3
Power Gasifier	72.2	70.7
Hydrogen Liquefaction	71.0	68.3
Energy Conversion	35.7	37.9
Overall	26.2	23.1

Thermal efficiencies of the feedstock and power gasifier sections are 58.6% and 72.2% respectively. These efficiencies are based on inputs of coal, fuel gas, and power and either crude hydrogen feedstock or fuel gas output. No other input or output streams have any thermal value.

The hydrogen liquefier, including the feedstock booster compressor and cryogenic purifier, has a thermal efficiency of 71.0%. The electrical energy input to the liquefier is computed on an equivalent electrical to thermal energy conversion of 3414 Btu/kwh.

The tabulation of thermal inputs and outputs at the bottom of Table 15 shows a higher output for the hydrogen liquefier than for the overall process. This is because the output of the liquefier includes a 560 MM Btu/hr item to account for the heating value of the tail gas. For the overall process, the tail gas is assumed to be recycled as fuel in the calculation of thermal efficiency in accordance with accounting rule No. 3. Its heating

value is therefore credited against overall thermal input.

The energy conversion section has a thermal efficiency of only 35.7% but this is typical for actual thermal to mechanical, or electrical, energy conversions. This section consists of gas turbines, fueled by the output fuel gas from the power gasifier and used to drive generators to produce electrical energy for internal consumption or for export to the hydrogen liquefaction complex.

The overall thermal efficiency of the complete plant from coal input to liquid hydrogen output is 26.2%. This low efficiency is the result, to a rather large extent, of the low efficiency of the energy conversion section, which takes as input about 48% of the combined output of the two gasifier sections and converts it at the aforementioned efficiency of about 36%. Any improvement in the performance of the gas turbines would be of particular benefit in the improvement of the overall process efficiency. An efficiency of 36%, however, is considered to be reasonable in today's gas turbine technology. Efficiencies in the low to mid forty percent are attainable with additional heat recovery equipment. Detailed attention to this area could improve the overall efficiency several percent.

A breakdown of the power consumption in the feedstock and power plant gasifiers is shown in Figure 39 for the base case.

Since a typical Eastern coal such as that used for the base case calculations will contain only from 4 to 6% moisture, coal drying is a relatively small energy consumer in the gasification process - less than 0.5% of the total energy consumption shown in Figure 39. In the base case the fuel for all coal drying is taken from the clean, low-Btu fuel gas produced by the power plant gasifier. Depending on the sulfur content of the

coal and the allowable sulfur emission levels, it would be possible to conserve some energy by obtaining a portion of the required drying energy by burning coal directly. However, even if all of the drying energy were obtained by burning coal directly, total coal requirements would be reduced by less than 0.3%.

The thermal efficiency of the gasifier is defined as the usable heat output in gas and steam divided by the total heat input to the gasifier. A K-T gasifier using a typical Eastern coal will have a thermal efficiency of 85 to 90 per cent. For the base case the thermal efficiency of the gasifier units alone, excluding subsequent compression, purification and shift conversion, is 89%. Since the heat input to the gasifiers is large (the heating value of the coal) even a small percentage loss in the gasifier becomes a significant part of the overall losses as shown in Figure 39.

Since sulfur removal in the base case is by a cold methanol absorption process using nitrogen (available from the oxygen plants) and flashing for regeneration, the power plant gasifiers require relatively little energy for acid-gas removal. However, the overall power requirement for acid-gas removal is increased by the necessity of removing the ${\rm CO}_2$ from the feedstock product gas using existing technology - hot carbonate absorbtion with steam regeneration. Possibilities for improvements in the area will be discussed later with the other areas that are judged to be critical development areas for process improvement.

Although the shift reaction itself is highly exothermic, the water gas shift section is a net energy consumer because of the heat used to generate the steam to drive the reaction. As in the case of the energy for drying, the energy for the steam generation comes from the clean, low-Btu

fuel produced by the power plant gasifiers. If a low sulfur coal which could be burned without gasification and treatment were available for use in steam generation, the total coal requirement for the system would be reduced by 3% if coal is used to generate steam for the water-gas shift section and by another 2% if the coal is used to generate the steam for the CO₂ removal also.

The largest source of inefficiency in the coal gasification sections is the power generation. The effects of improved power conversion efficiencies as well as the effects of developing a high pressure K-T gasifier to reduce compression requirements will be discussed later with other critical areas for future process development.

2. OTHER FUELS

Thermal efficiencies for the production of possible alternate fuels for jet aircraft consumption have been determined from published information. Fuels which were considered are:

- Liquefied natural gas (LNG) by liquefaction of SNG produced via the Lurgi coal gasification process.
- Methanol via conventional high pressure synthesis using synthesis gas generated by steam reforming of natural gas.

a. LIQUEFIED NATURAL GAS

Published power requirements for liquefaction of natural gas for the Phillips-Marathon oil liquefaction plant at Kenai, Alaska are presented by Peterson (9) and a plant description is provided by Culbertson and Horn (10). This plant was selected because the natural gas feedstock is nearly pure (99⁺%) methane. It is presumed that a similar liquefaction unit is fed by a Lurgi plant producing SNG, as described by Shaw and Magee (8).

Energy inputs and outputs used in deriving the thermal efficiency are listed in Table 16. The overall efficiency from coal to product LNG is 55.6%. The calculation presumes that by-products of the Lurgi process with useful fuel value are recycled as fuel; phenol, ammonia and sulfur are excluded from the calculation. The published data for power requirement of the liquefaction plant covers only the compressor power. While this represents the major power requirement, there are other requirements which must normally be provided for. To cover these, an arbitrarily assumed addition of 8% of the compressor power was taken.

The data for the Lurgi-SNG plant includes enough power for compression of the product gas to 900 psig. The liquefaction plant data are for a 650 psig natural gas feedstock. Calculation of the thermal efficiency for the combined operations credits the process for this pressure discrepancy.

The thermal efficiency of the LNG liquefier is very high compared with the hydrogen liquefier for several reasons. One is that hydrogen inherently requires greater work for liquefaction because of the lower liquefaction temperature. More important is that hydrogen has a heating value only 32% (vol. basis) of that for methane so that each Btu required for liquefaction consumes a greater percentage of the feedstock Btu's. Also contributing is the high thermodynamic efficiency of the cascade cycle used for LNG liquefaction which, for this example, calculates to be 43.6% compared with 36.0% for the hydrogen liquefier (Table 11). A cascade cycle is impractical for hydrogen liquefaction because the only possible working fluid below the liquid nitrogen temperature range is neon which, for this purpose, is unplentiful and costly.

b. METHANOL

Several publications (11, 12, 13, 14) list energy requirements for the production of methanol. The one selected (14) gives typical requirements for high pressure production of a synthesis gas via stream reforming of natural gas. Table 17 presents a summary of the thermal data. The 53.8% thermal efficiency is only slightly lower than that for LNG.

The heat in the product methanol is based on its higher heating value. There is no way of knowing the basis for the heat provided by the natural gas feedstock. There is some reason to believe that the 38 MM Btu/ton are actual process heat requirements and, if so, should be based on the lower or net heating value. In this event, the thermal efficiency would be lowered to 48.5%, assuming the natural gas is pure methane.

The process for production of methanol uses the rather highly efficient steam reforming process for production of the synthesis gas. For an equitable comparison, the synthesis gas should be produced via coal gasification which has a thermal efficiency 15 to 25 percentage points lower than for steam reforming. Methanol synthesis via gasification of coal might then be expected to have an overall thermal efficiency of 35% to 45%.

3. HEATING VALUES

The following tabulation lists both gross and net heating values for the various process streams.

HEATING VALUES

	Net	<u></u>	Gross	
	Btu/SCF	Btu/lb	Btu/SCF	Btu/lb_
Coal		12,000		12,500
Crude H ₂	261	33,230	308	39,240
Product H ₂	269	51,623	. 318.5	61,000
Tail Gas	187	4,860	209	5,430
Fuel Gas	27 5	5,445	292	5,790

VI. ECONOMICS OF LIQUID HYDROGEN PRODUCTION

A. SCOPE

Investment and operating costs are presented for the actual base case (1974) for the complete hydrogen production and liquefaction facility including all necessary power generation for the production of 2500 tons per day of 97% para liquid hydrogen. The total facility is divided into two separate and distinct units 1) the coal gasification unit and 2) the liquefaction complex; separate economics are reported for each unit which are subsequently combined to give total cost. Geographical considerations make this a realistic treatment inasmuch as the coal gasification complex is likely to be located at or near the mine site while the liquefaction complex will probably be located in reasonable proximity to the airport which it serves. Such logistic studies, although they are important, do not form a part of the present study. Therefore the means of transporting the necessary raw materials, intermediate products, final products or energy are not included in the study. It is assumed that the coal gasification unit generates crude hydrogen feedstock which is delivered, under pressure, to a pipeline and that the hydrogen is removed from the pipeline at the liquefaction site at the same process conditions as it entered. Similarly, electrical energy is generated from gaseous fuel via gas turbine driven generators at the coal gasification site and is made available at the liquefaction site without regard to transmission requirements.

The economics of liquid hydrogen production in the 1985-2000 time frame are projected from 1974 economics and technology. Costs are reported in mid-1974 dollars in all cases. The areas of development which are considered for future technology are evaluated with respect to their economic impact on current technology. Cost adjustments to estimates for the actual base case (1974) are then made to arrive at actual costs for production and liquefaction of hydrogen in the years 1985-2000.

B. FINANCING METHODS:

Unit hydrogen costs were calculated on a dollars-per-pound basis for the liquid hydrogen product. This is done for both the gasification and liquefaction complexes and for the sum of the two to arrive at a total unit cost.

Financing methods were determined on both a Discounted Cash Flow (DCF) basis, which is representative of industrial financing, and on a public utility basis; results from both methods are presented. The calculation procedure for the public utility method is that developed by the American Gas Association General Accounting Committee (23) and later modified slightly by the Panhandle Eastern Pipeline Company. These are the same methods adopted by the Synthetic Gas-Coal Task Force for estimating cost of manufacturing SNG from coal. Shortcut equations used in cost determination are given in Tables 18 and 19 where actual calculations and the basis for same are also presented for DCF and utility financing respectively.

C. LIQUEFACTION ECONOMICS

Capital investment requirements for the actual base case (1974)
2500 TPD liquefaction complex are presented in Table 20. Included is
\$528,197,000 total plant investment for a grass roots facility consisting
of the hydrogen liquefier, cryogenic purifier, feed and booster compressor,
and all on site auxiliary equipment in an installed and operating condition.
Additional capital requirements include interest on total plant investment
during construction, startup costs and working capital to bring the total
capital requirement to nearly \$650 million.

Annual operating cost for the same facility is presented in Table 21; only costs associated with operation of the liquefaction unit are considered. No charge is made for the hydrogen feedstock stream nor the electrical energy since these are provided by the coal gasification complex. Total operating cost is \$29,348,900 annually which is equal to a unit cost of 1.69 \$/lb of hydrogen product.

Total unit liquefaction costs are presented in Tables 18 and 19 for DCF and utility financing, respectively. These are 9.20¢/lb based on DCF method and 6.20¢/lb for a utility-financed project.

D. LIQUEFACTION COST - 1985/2000 TIME PERIOD

Applying the cost benefit factors described in Section VII entitled

"Areas of Development Opportunity - 1985/2000 Time Period", unit liquefaction

costs are derived. These are shown in Table 22. Net impact of the future

liquefaction developments is to decrease the unit cost of liquefaction by

6% for both methods of financing.

E. GASIFICATION ECONOMICS

Capital investment requirements for the actual base case (1974) 2500 TPD coal gasification complex are presented in Table 23. This table also shows the estimated investment for the 1985/2000 time period which can be expected with the successful completion of the development efforts outlined in the report section entitled "Areas of Development Opportunity." The total plant investment of \$1,540,800,000 includes all operating areas as listed and covers all necessary items for installation of a grass roots facility with the exception of the acquisition of land. The investment requirements of the liquefaction complex are not listed here; these can be found in Table 20.

The gasification complex has two major functions: 1) to provide hydrogen feedstock for the liquefier and 2) to generate the necessary power for operation of both the liquefier and the hydrogen generator. The power generating section is the larger of the two, requiring 63% of the total plant investment.

Total plant investment for the future time period is estimated to be \$1,142,800,000, a reduction of more than 25% from the 1974 estimate. The future developments have a greater impact on reducing energy and power requirements than on reducing feedstock requirements. This is shown in a breakdown of costs between power and feedstock generating sections where the investment in the power generating section for the future plant is reduced to 57% of the total.

Total unit gasification costs are presented in Table 24 based on DCF financing and in Table 25 based on utility financing. Economics based on three different values (35, 50 and 75¢/MM Btu) for the cost of coal are shown. Equivalent costs for a 12,000 Btu/lb coal are \$8.40, \$12.00 and \$18.00 per ton respectively. Working capital and startup costs are a function of the cost of coal and vary with it. Unit cost for gasification varies from 27.50 to 37.78 ¢/lb for utility financing and 36.20 to 46.64 ¢/lb for DCF.

Future unit cost of gasification is expected to be about 25% lower than present cost for both financing methods.

The unit costs shown in Tables 24 and 25 are solely for gasification. To these must be added the cost of liquefaction to obtain the total unit cost for liquid hydrogen. This has been done in Table 26 which shows the 1974 cost of hydrogen to vary from 33.70 to 43.98 \$/lb based on utility financing and 45.40 to 55.82 \$/lb for DCF financing. Future costs are about 21-22% lower for both financing methods.

Total unit costs are also presented graphically in Figure 40.

It is apparent that the cost of liquid hydrogen is only moderately affected by the cost of coal. A 150% increase in coal cost produces only a 31% increase in hydrogen cost for a utility-financed project and a 23% increase for DCF financing. It is also apparent that the sensitivity will be even slightly less in the 1985-2000 future time period.

Costs given in Table 23, represent the total of the costs (calculated separately) of the feedstock gasification and the power plant gasification sections. For the base case, the feedstock gasification section is not independent (see Section IV-A) since it requires the equivalent of approximately 34% of the fuel gas output of the power plant gasifiers. If it is assumed that the cost of the overall gasification complex is relatively unchanged with a different division of the major sections of the plant, appropriate percentages of the costs of the components of the power plant may be allocated to the feedstock gasifiers so that a rough estimate of the cost of a self-sufficient feedstock gasification system may be obtained. Approximate Total Plant Investments (see Table 23) for an independent feedstock gasification section would be \$872,000,000 and \$706,000,000, respectively, for 1974 and for the future time period. Unit costs of gaseous hydrogen from such a system would be as follows:

Cost of Gaseous Hydrogen Feedstock, c/lk				ock, ¢/lb		
	1974		1985-2000			
Coal Cost (1)	0.35	0.50	0.75	0.35	0.50	0.75
Financing						
DCF	21	23	27	17	19	22
Utility	16	18	22	13	15	18

^{(1) \$/}MM Btu

VII. AREAS OF DEVELOPMENT OPPORTUNITY: 1985-2000 TIME PERIOD

A. LIQUEFACTION

1. Improved Compression Equipment

The thermodynamic analysis showed that nearly 53% of the total energy losses in the work of liquefaction occurred because of compressor inefficiencies. Therefore, any improvement in compressor performance should lead to significant saving. Unfortunately such improvement may be rather difficult to achieve because of the highly developed state of the art in compressor technology. Adiabatic efficiencies used in the parametric study for compression equipment varied from 65% to 80% with the bulk of the compression occurring at 80%, including both centrifugal and reciprocating machines. These are realistic values for large present day compressors and somewhat easier to achieve in the reciprocating than in the centrifugal types. Nevertheless it may be possible to increase efficiencies by perhaps 3 percentage points by a suitable development effort.

With reciprocating compressors, piston blow-by losses occur and these contribute to inefficiency. Opportunities for a decrease of piston blow-by lie in development of lighter pistons which would permit higher piston speeds and shorter gas residence time in the cylinder. Titanium, for example, as a material of construction would typically provide a lighter piston. Development of new materials such as new lubricants and new types of piston rings would provide better sealing and reduce blow-by.

A valve development effort might permit use of larger valve areas which would add to compressor efficiency.

A reciprocating compressor operating at higher speeds would also result in smaller cylinders for a given capacity and would offer some opportunities for investment reduction.

The investment in the reciprocating compressors is a significant item, amounting to approximately 30% of the total purchase price of equipment in the liquefaction complex. A centrifugal compressor in the same service would require much lower investment. With present day technology, however, hydrogen cannot be effectively compressed by centrifugal methods. The difficulty arises from the low molecular weight of the hydrogen, and the resulting low density, which produces an extremely high adiabatic head. Even applying the maximum possible adiabatic head per stage with present technology, the resulting compressors would have an excessively large number of wheels. There are currently studies being made on high speed, high head wheels which could possibly develop into a practical centrifugal compressor for hydrogen service but the chances for success must be considered conjecture as of now.

Nearly all the compression development work being conducted at the present time is on centrifugal equipment. There is a declining interest in large reciprocating compressors because in most applications the centrifugal compressor can do the same job at lower investment, if not equal efficiency.

It is therefore unlikely that there will be any development effort on reciprocating compressors in the private sector of the economy unless it is publicly financed. Alternatively, private interest would well be stimulated by the large market which would arise out of the successful implementation of a liquid hydrogen fuels program.

For the 1985-2000 time frame, it is assumed that successful compressor development will result in an improvement in compressor efficiency amounting to 3 percentage points for both reciprocating and centrifugal compressors. This results in a power requirement which is 96% of that for the actual base case (1974).

2. Improved Hydrogen Expanders

The thermodynamic losses in the hydrogen turbines amount to about 19% of total liquefaction losses. This performance was based on a 79% isentropic efficiency, which is perhaps somewhat conservative. With some development work and design optimization centered around seal improvement and nozzle design, improved performance at 85% efficiency is not unreasonable. Examples of commercially installed turbines with better than 85% isentropic efficiency in present day technology are known.

For the 1985-2000 time frame, an isentropic efficiency of 85% is assumed resulting in a power requirement which is 96% of that for the actual base case (1974).

3. Partial Ortho-Para Conversion

This concept offers the greatest opportunity for reduced liquefaction power consumption. Very little development work is required for implementation.

The major uncertainty is whether, in a practical, commercial operating system, the reaction rate for the autoconversion is identical to the purely uncatalyzed rate. Some materials of construction used in storage and distribution equipment may have a possible catalytic effect which would distort present results deleteriously.

Aside from extraneous catalytic action, successful application depends upon logistics and consumption patterns. Production and consumption schedules must be synchronized to permit the product to be utilized shortly after it has been liquefied. The more perfect the synchronization, the shorter the period of time that the product will exist in its liquid state, the lower the required para content, and the lower the required power.

For the 1985-2000 time frame, it is assumed that extraneous catalytic activity does not exist and that a rather generous 50-hour period is representative of the maximum elapsed time between liquefaction and consumption of product. Figure 4 gives a 60% pH $_2$ composition required for a 50-hour breakeven time. For 60% pH $_2$, the energy requirement, according to Figure 14, is only 87% as great as for the actual base case (1974).

4. <u>Hydrogen Leakage Reduction</u>

Another development which would require a minimum of development and which would almost certainly result in successful implementation lies in the area of reduction of leakage losses. Pure hydrogen at the liquefaction stage has undergone a considerable amount of costly processing and warrants

a concerted effort toward conservation. Hydrogen flow in the liquefier recycle loop amounts to nearly 5 times the product flow so that compressor leakage losses are effectively multiplied by a factor of 5 with respect to product flow.

Total allowance for loss of hydrogen in the liquefaction complex amounts to about 14%. Not all this is due to compressor leakage: losses resulting from storage tank leakage and evaporation, process equipment leakage, purifier purge and vent and purifier stripping requirements are included. The compression leakage losses amount to about 5%.

Collection devices at the piston rod seals will permit recovery of a large portion of the leakage loss and will reduce feedstock requirements if not compression power requirements.

The use of lubricated compressors can also be considered. This would reduce leakage losses, to the range of a fraction of one percent if special lubricants are used. Of course, suitable lubricant removal systems must be developed and employed in the process.

Recovery and recycling of evaporation losses will further reduce feed stock requirements.

For the 1985-2000 time frame, it was assumed that 90% of the leakage loss from the compressors was recovered and that 50% of storage losses rather than 20% was recovered. Total effect is a 4.6% reduction in feedstock requirement compared with the actual base case (1974).

5. Purifier Tail Gas Utilization

Hydrogen comprises about 45% of the tail gas, which is a by-product of the cryogenic purification process. Utilization of this gas for fuel purposes was adopted for the actual base case resulting in a loss of 2.6% of the hydrogen contained in the feedstock.

Hydrogen recovery via cryogenic processing can be profitably applied in this case; value of the hydrogen recovered would exceed, by a wide margin, the required investment in the cryogenic processor. The remaining tail gas would still have fuel value but some make up power from the coal gasification unit would be required to replace the fuel value of the recovered hydrogen.

For the 1985-2000 time frame, it was assumed that 80% of the hydrogen in the tail gas stream was recoverable. This permitted a 2.1% reduction in hydrogen feedstock to the liquefaction complex but a 2.1% increase in power was required over the actual base case (1974).

6. Combined Effects

Summarizing the individual gains of the preceding sections:

<u>Power</u>

	% of Base Case
Improved Compressors	96
Improved Hydrogen Expanders	96
Partial Ortho-Para Conversion	87
Tail Gas H ₂ Recovery	102.1
Combined Effect	81.9

Feedstock	% of Base Case
Leakage Reduction	95.4
Tail Gas H ₂ Recovery	<u>97.9</u>
Combined Effect	93.4

In the 1985-2000 time period, the total power required for the liquefaction complex is 81.9% of the 1974 actual base case, while the feedstock requirements are only 93.4% as great for the same production capacity.

Investment estimates show an overall reduction of 6% resulting largely from the decrease in compression requirements. The effect of these reductions on overall plant performance and cost is treated in Section VI on economics.

B. GASIFICATION

The K-T gasifiers of the base case operate at a slight positive pressure above atmospheric, but the gas purification (H₂S and CO₂ removal) processes require a considerable pressure to operate effectively. Even if these processes did not require pressure, both the liquefier section and the gas turbines operate with compressed gases so that somewhere in the gasification system the pressure must be increased above atmospheric. A K-T gasifier operating at medium to high pressures could provide significant savings in energy requirements if such a gasifier could be developed. The complexity and increased cost of a pressurized gasifier with the necessary system for feeding coal under pressure would be offset by the decreased costs

and greater simplicity of the processes downstream of the gasifier. Extra power needed to feed in the coal under pressure would be more than offset by the 71% reduction in gas compression work caused by eliminating the raw gas compressors and adding oxygen compressors to compress the oxygen for the gasifiers. The heat recovery systems after the gasifiers could be made much more compact because of the higher density of the pressurized raw gas. Pressure drops in heat exchangers would be less of a problem. In the base case the raw gas is cooled and then compressed. The heat added to the gas by the compression must then be removed before the gas goes to the sulfur removal section. If the pressurization occurs in the gasifier, this second cooling step would be eliminated.

The processing steps of the base case must be carried out in a definite sequence because of the limitations of the different steps. The raw gas must be cooled, compressed, cooled again for sulfur removal, and then reheated for the shift reaction. As discussed before, a high pressure K-T would eliminate some of the heat exchange systems. Also, different purification systems and changes to existing systems should be considered for future hydrogen generation facilities. Although the reaction itself is exothermic, the water gas shift section is an energy consumer since the raw gas, aftercooling and sulfur removal, does not contain nearly enough water to drive the reaction. If a shift catalyst which could operate effectively in the presence of sulfur could be developed in conjunction with

a high pressure gasifier, steam addition for the water gas shift could be decreased if the reaction were carried out before cooling the gas and removing water from it. An alternative to this would be to develop a high temperature sulfur removal system which also would eliminate part of the heat exchange requirements of the base case.

The CO_2 removal system is a major energy consumer because of its need for steam for regeneration. A method of decreasing energy consumption for acid gas removal would be beneficial. One way would be by the use of a dual-purpose system which would be effective for $\mathrm{H}_2\mathrm{S}$ and CO_2 . Since hot carbonate processes can be used to remove $\mathrm{H}_2\mathrm{S}$ as well as CO_2 (22), the feedstock gasification section could be simplified by using a single acid-gas removal process to remove $\mathrm{H}_2\mathrm{S}$ before the shift and CO_2 after the shift.

Figures 39 and 41 show the total effect that several possible future developments would have on energy and economic requirements of a hydrogen liquefaction facility. Future development work is assumed to cause the following improvements in the hydrogen liquefaction facility:

1. An increase of 2 to 3 percentage points in gas turbine and steam turbine efficiencies - Although steam turbines are already well developed, an increase in efficiency is based on the assumption that energy conservation measures required by energy shortages will be an incentive to the development of even more efficient steam turbines. Improved design, better heat recovery, and larger sizes (such as would be required by a 2500 TPD H₂ plant) will improve gas turbine efficiencies.

- 2. A 17% decrease in power requirement and a 20% decrease in investment for large oxygen plants resulting from development of specialized, highly efficient air separation process directed toward coal gasification applications, and from development of new and improved construction techniques.
- 3. A 40% decrease in energy requirement for ${\rm CO_2}$ removal resulting from development of a dual system for removing both ${\rm H_2S}$ and ${\rm CO_2}$.
- 4. Improvements in the liquefaction process as discussed in the previous section.

VIII. AREAS FOR ADDITIONAL STUDY

A. GASIFICATION

1. Commercial Gasifiers and Potential Modifications

Most of the coal gasification work has been concentrated upon SNG production. A more thorough analysis of hydrogen production is desired. This can be done utilizing the work to date as a yardstick for performance rating. First, two additional studies should be made on the K-T gasifier. The initial study is a second law analysis to determine the areas in which the low pressure gasifier can be improved. The second is to anticipate that a high pressure K-T gasifier can be developed. Next, the Lurgi gasifier should be examined for another point of reference. Finally, the combination of K-T and Lurgi gasifiers might be applied, one type for H₂ production and the other for fuel gas.

Advanced Gasifier and Coal Converters

Two advanced gasifier systems are suggested for advanced hydrogen production studies: the CO_2 -acceptor process and the UCC agglomerated bed process. The CO_2 -acceptor process is chosen because the exothermic acceptor reaction

also drives the water gas shift

$$CO + H_2O \implies H_2 + CO_2$$

thus offering an opportunity to save steam. This thermodynamic leverage is unique among all the advanced coal gasification processes. The UCC

agglomerated bed process is typical of most advanced coal gasification processes and has been chosen here for comparison because of available information by the Linde Division.

The final advanced coal conversion process recommended for study is the Solvent Refined Coal Process. This process is applied along with other gasification processes to produce hydrogen. Here, a sulfur-free raw material would be made available which could be most attractive because of logistics flexibility and coal feeding. SRC can be heated to a liquid form and be more readily fed to gasifiers operating under pressure than ordinary coal. Thus, this would offer also great flexibility in the type of gasifier that can be used for hydrogen production. Fuel gas generation would not be necessary because the fuel is sulfur free and the heating value is about 14,500 Btu/lb as compared with 8,000 to 13,000 Btu/lb for coal. SRC gives the option of taking some of the inefficiencies at the coal mine and SRC processing plant, before gasification for hydrogen production or before direct combustion for power generation. The impact of SRC should be investigated in terms of flexibility for logistics purposes and liquid hydrogen production.

B. PURIFICATION

A substantial portion of the capital investment is connected with hydrogen purification. It would be appropriate to conduct a survey of existing H_2S and CO_2 removal systems which can be best integrated with final cryogenic purification prior to hydrogen liquefaction. Special attention

will be given to H_2S/CO_2 selectivity for sulfur rejection and the minimization of steam usage in solvent regeneration. The overall objective will be to tailor the purification process for optimum performance and economics with coal as the original hydrogen producing feed stock.

C. LIQUEFACTION

1. Partial Ortho-Para Conversion

Because this appears to be the most likely approach to substantial reduction in energy requirement for hydrogen liquefaction it deserves additional attention and study to determine the practicality of the concept. This would consist of at least an in-depth survey of existing literature data on the catalysis of the ortho-para reaction. If necessary, additional experimental work should be undertaken to determine whether common materials of construction such as aluminum, copper and copper alloys, and austinitic stainless steels have any effect on the conversion rate.

2. Wet Turbines and Ejectors

This recommendation is for additional process studies on the hydrogen liquefier process. The subcooled hydrogen product emerges from the final converter under nearly full feed pressure at about 28°K and is then passed through a throttling valve which results in a slight rise in temperature. The product stream then passes through a small trim-converter to a subcooling heat exchanger where it is cooled to near boiling point temperature by means of boiling low pressure refrigerant hydrogen. A wet turbine substituted for the

throttling valve could be a valuable process addition because it would reduce the amount of refrigeration that has to be supplied by the low pressure hydrogen.

The temperature of the hydrogen product emerging from the final converter is limited by the saturation temperature of the exhaust stream from the low temperature turbine at the discharge pressure. This temperature can be lowered by reducing the discharge pressure but now the recycle return streams are at 2 different pressure levels which adds process complexity. The lower pressure also causes an increased pressure loss in the return stream which increases equipment requirements or process power or both. An ejector could possibly be inserted in the process in such a way as to use the exhaust from the warm turbine as the motive stream to raise the pressure of the exhaust from the cold turbine. The combined streams from the ejector would be recycled as usual.

Both of the preceding process variations offer possibilities for process improvement and warrant additional study.

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TABLE 1
THEORETICAL WORK FOR LIQUEFACTION
OF HYDROGEN

FOR 99.8% PARA $\rm H_2$

PROCESS	CONVERSION STAGE TEMPERATURES, °K	WORK <u>KWH/LB</u> •	<u>RELATIVE</u>
1. REVERSIBLE	N.A.	1.799	1.000
2. STAGEWISE PLUS REVERSIBLE	110	1.803	1.002
3. STAGEWISE PLUS REVERSIBLE	80	1.817	1.010
4. STAGEWISE (5 STAGES)	80, 65, 50, 35, 20.23	1.922	1.068
5. STAGEWISE (4 STAGES)	80, 60, 40, 20.23	1.961	1.090
6. STAGEWISE (3 STAGES)	80, 50, 20.23	1.983	1.102
7. STAGEWISE (2 STAGES)	80, 20.23	2.209	1.228
8. STAGEWISE (1 STAGE)	20.23	2.439	1.356
FOR NORMAL H ₂ (25% PARA)			
9. NO CONVERSION		1.523	0.847
FOR 80 °K EQUILIBRIUM H ₂ (.48.54	% PARA)		
10. STAGEWISE	80°	1.581	0.879

Note: Feed is normal H_2 at 1 atm and 300 °K

Product is liquid H_2 at 1 atm and 20.23 °K

Heat rejection temperature = 300 °K

Thermodynamic data for H_2 from Hall et al (2)

Kilojoule/gm = 7.9367 (KWH/LB)

TABLE 2

LIST OF PROCESS PARAMETERS

FOR PARAMETRIC STUDY

OF HYDROGEN LIQUEFIER

	PARAMETER	PROCESS LOCATION (1)	FIGURE NO.(3)
1.	HYDROGEN FEED PRESSURE	1	9
2.	RECYCLE BACK PRESSURE	60	10
3.	MINIMUM REFRIGERATION LEVEL	29	11
4.	EXPANDER EFFICIENCY	E-1, E-2	12
5.	COMPRESSOR EFFICIENCY	P-RC, P-SCF (2)	13
6.	PARA CONTENT	19	14
7.	WARM END TEMPERATURE APPROACH	X-1, X-8	15
8.	WARM END TEMPERATURE APPROACH	XC-3, X-3	16
9.	COLD END TEMPERATURE APPROACH	XC-2, X-2	17
10.	REFRIGERATION ARRANGEMENT		18

- (1) REFERS TO STREAM OR EQUIPMENT NUMBER FIGURE 7.
- (2) INCLUDES ALSO, HYDROGEN FEED COMPRESSOR AND ALL NITROGEN COMPRESSORS OF NITROGEN LIQUEFIER.
- (3) PERFORMANCE CURVES.

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TABLE 3

PROCESS STREAM CONDITIONS - HE LIQUEFIER

800 5FQ = 213 *** BEGIN P	PRINT					
STREAM NO N-(STYP/KTYP/HTYP)	080(01/01/01)	081(01/01/01)	082(0]/01/01)	083(01/01/01)	084(01/01/01)	085(01/01/01)
_	2573154	3573150.	3573150.	845711.	845711.	665672.
FLOW+ CFH(NTP)f	3573150.	9237.96	9237.96	2186.49	2186.49	1721.02
FLOW: LP:MOLE/HR FM	9237.96		84.0000	600.000	22.0000	22.0000
PRESSURF + PSIA P	90.0000	90.0000	299.919	99.9000	81.0186	81.0186
TEMPERATURE. DEG K T	97.0000	300.000	_	942.897	942,896	444.204
FNTHALPY+ BTU/LB.MOLE H	2879.48	5553.63	5553.63	11.0117	12.3449	6.19041
ENTROPY. RTU/LB.MOLE-DEG K S	31.6080	46.7331	46.9795	· · · - ·	0.787115	SAT. LIQ
I IQUID FRACTION (L/F) PL	S.H. VAP	5.H. VAP	S.H. VAP	S.C. LIQ	4.191112	3711 2.4
COMPOSITION. MOLF FRACTION:						1,000000
NITROGEN X1	1.000000	1.000000	1.000000	1.000000	1.000000	1400000
		•.				
			- Committee of the second	 		
(22)						
	004 (01 (01 (01)	087(01/01/01)	088(01/01/01)	089(01/01/01)	090(01/01/01)	091(01/01/01)
STREAM NO N-(STYP/KTYP/HTYP)	086(01/01/01)	001(01)01)	, , , , , , , , , , , , , , , , , , , ,			
	307394.	307394.	358278.	358278.	180039.	845711.
FLOW. CFH(NTP) F	794.731	794.731	926.286	926.286	465.469	2186.49
FLOW+ LP+MOLE/HR FM		22.0000	22.0000	22.0000	22.0000	22.0000
PRESSURF + PSIA P	22.0000	81.0186	81.0186	81.0186	81.0186	81.0186
TEMPERATURE. DEG K T	81.0186		444.204	2786.75	2786.75	2786.75
ENTHALPY: BTU/LB.MOLF . H	444.204	2786.75	6.19041	35.1003	35.1003	35.1003
ENTROPY. BTU/LB.MOLE-DEG K S	6.19041	35.1003		SAT. VAP	SAT. VAP	SAT. VAP
LIQUID FRACTION (L/F) PL	SAT. LIG	SAT. VAP	SAT. LIQ	SHIT THE		
COMPOSITION, MOLF FRACTION:				1.000000	1.000000	1.000000
NITROGEN X1	1.000000	1.000000	1.000000	1.000000	1,000,000	
			•	•		
			•			'
STREAM NO. + N-(STYP/KTYP/HTYP)	092(01/01/01)	093(01/01/01)	094(01/01/01)	095(01/01/01)	096(01/01/01)	
···	221920.	221920.	1067630.	1067630.	1067630.	
FLOW + CFH(NTP) F	_ _	573.748	2760.23	2760.23	2760.23	
FLOW+ LA-MOLF/HR FM	573.748	· · · · ·	22.0000	22.0000	15.0000	
PRESSURF + PSIA P	22.0000	22,0000	82.9978	300.000	299.904	•
TEMPERATURE. DEG K T	90.6000	90.6000	2813.17	5565.23	5565.23	
ENTHALPY: ATU/LB_MOLE H	2913.85	2913.85	- 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1 - 1		53.1732	
ENTROPY. RTU/LB.MOLE-DEG K S	36.5832	36.5832		S.H. VAP	S.H. VAP	•
LIQUID FRACTION (L/F) PL	S.H. VAP	S.H. VAP	S.H. VAP	Same AME		
COMPOSITION. MOLF FRACTION:			1 000000	1.000000	1.000000	
NITROGEN X1	1.000000	1.000000	1.000000	1.00000	200000	

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-	STREAM NO. N- (STYP/KTYP/HTYP	> }	001(04/01/01)	002(04/01/01)	003(04/01/01)	004(04/01/01)	005(04/01/01)	006(04/01/01)
	STACEN NOTE IN THE				1227875.	20119088.	20119088.	1724758.
	FLOW+ CFH(NTP)	F	400000.	2772125.		52015.6	52015.6	4459.16
		FM	10341.5	7167.00	3174.53	600.000	600.000	600.000
	FLOW. LR.MOLEZHR	Þ	600.000	600.000	600.000		85.5000	85.5000
	PRESSURF + PSIA	Ť	308.000	308.000	308.000	308.000	1160.32	1160.32
	TEMPERATURE. DEG K	i.	3776.98	3776.98	3776.98	3776.98	33.3969	33.3970
	ENTHALPY. BTU/LB.MOLE	_	48.3138	48.3138	48.3138	48.3138		S.H. VAP
	ENTROPY. RTU/LB.MOLE+DEG K	. >		S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	34H4 YAC
	I TOUTD FRACTION (L/F)	PL	S.H. VAP	Selle TAP	3			
	COMPOSITION. MOLF FRACTION:		_	. 75.000	0.750000	0.750000	0.750000	0.750000
	ORTHO-HYDROGEN	X1	0.750000	0.750000		0.250000	0.250000	0.250000
		X2	0.250000	0.250000	0.250000	0,25000		
	PARA -HYDROGEN	~-		,				
			•			The second secon		
			and the second of the second		•			
								012(04/01/01)
	T			008(04/01/01)	009(04/01/01)	010(04/01/01)	011(04/01/01)	015(04/01/01)
	STREAM NO. + N-ISTYP/KTYP/HTY	P)	007(04/01/01)	008(04/01/01)			•	
	- SINERII IIOTI II III II				21843840.	4000000.	4000000	4000000-
	FLOW+ CFH(NTP)	F	21843840•	4000000 <u>.</u>		10341.5	10341.5	10341.5
		FM	56474.7	10341.5	56474.7	598.500	598.500	586.000
	FLOW: LA.MOLE/HR		600.000	600.000	598,500		81.2186	81.1027
	PRESSURF + PSIA	Ţ	85.5000	308.000	85.4874	85.4874	991.899	991.898
	TEMPERATURE. DEG K		1160.32	0.0	1160.32	1160.32		31.8115
	ENTHALPY+ BTU/LB.MOLE	H		0.0	33.4050	33,4050	31.7425	S.H. VAP
	ENTROPY. ATU/LB.MOLE-DEG K	S	33.3969	SAT. VAP	S.H. VAP	S.H. VAP	S.H. VAP	2.U. AWL
	LIQUID FRACTION (L/F)	PL	S.H. VAP	SAI. YAF	3,110			
	COMPOSITION. MOLE FRACTION:		_	يدين والمراجعين		0.750000	0.545095	0.545095
		X1 -	0.750000	0.750000	0.750000	0.250000	0.454905	0.454905
	ORTHO-HYDROGEN	X2	0.250000	0.250000	0.250000	0.25000	• • • • • • • • • • • • • • • • • • • •	
	PARA -HYDROGEN	A.L	•••					-
						•		
	•			•				
								018(04/01/01)
				014(04/01/01)	015(04/01/01)	016(04/01/01)	017(04/01/01)	019(04)01)01)
	STREAM NO N-(STYP/KTYP/HT)	(P)	013(04/01/01)	014(04/01/01/	0101047041	-		
	JINEMII NOO				4000000.	4000000.	4000000-	4000000
	ELOU CENTAL	F	4000000	4000000		10341.5	10341.5	10341.5
	FLOW+ CFH(NTP)	FM	10341.5	10341.5	10341.5	571.000	135.000	135.000
	FLOW. LR.MOLE/HR	FM	586.000	578.500	578.500		28.6723	29.0895
	PRESSURF + PSTA	_	41.1735	41.1035	28.0000.	28.0281	-	-94.7838
	TEMPERATURE. DEG K	ł		202.673	-94.7814	-94.7821	-94.7836	11.571/
•	FNTHALPY. BTU/LB.MOLE	н	202.674	18.2160	10.0658	10.0897	11.5706	
	ENTROPY. BTU/LB.MOLE-DEG K	5	18.1844		S.C. LIQ	S.C. LIQ	5.C. L10	S.C. LII
	LIQUID FRACTION (L/F)	PL	S.C. LIQ.	s.C. L10	2**** ****		rangement to other to the	,
	LINDIO PARCITON (E.)					0.041322	0.041322	0.03029
	COMPOSITION. MOLE FRACTION:	X1	0.205956	0.205956	0.041322		0.958678	0.96971
	ORTHO-HYDROGEN	_	0.794044	0.794044	0.958678	0.958678	V = 250010	
	PARA -HYDROGEN ,	X2						•
			•					

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STREAM NO N-(STYP/KTYP/HTYP)	019(04/01/01)	020(04/01/01)	021(04/01/01)	022(04/01/01)	023(04/01/01)	024(04/01/01)
_	4000000	17843856.	17843856.	17843856.	6751505.	6751505.
FLOW • CFH(NTP) F	10341.5	46133.2	46133.2	46133.2	17455.2	17455.2
TEORY Englished the	135.000	598.500	598.500	596.000	596.000	50.0000
PRESSURF + PSIA P	20.5700	85.4874	81.2186	81.1955	81.1955	39.1735
TEMPERATURE + DEG K T	-194.070	1160.32	1113.28	1113.28	1113.28	784.596
ENTHALPY - RTU/LB . MOLE . H	7.60710	33.4050	32.8499	32.8631	32.8631	35.2904
ENTROPY. BTU/LB.MOLE-DEG K S		S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP
LIQUID FRACTION (L/F) PL COMPOSITION:	S.C. LIG	3+H+ YAF	Dent ter	3,110 (111	•	
ORTHO-HYDROGEN XI	0.030290	0.750000	0.750000	0.750000	0.750000	0.750000
PARA -HYDROGEN X2	0.969710	0.250000	0.250000	0.250000	0.250000	0.250000
PARA -HYDROGEN X2	, , , , , , ,		•••			•
7						
60		40403 .031	A37 (A4 (A) (A))	028(04/01/01)	029(04/01/01)	030(04/01/01)
STREAM_NO N-(STYP/KTYP/HTYP)_	025(04/01/01)	026(04/01/01)	027(04/01/01)	060104/01/01/	42714 77 41741 7	
FLOW CEHINTP)	11092371.	11092371.	10456493.	10456493.	10456493.	635878.
12001	28678.0	28678.0	27034.0	27034.0	27034.0	1643.49
_ redar Engineering	596.000	596.000	596.000	596,000	52.0000	596.000
PRESSURF PSIA P	81.1955	58.3915	58.3915	58.3915	26.0000	58.3915
TEMPERATURE DEG K T	1113.28	836.741	836.741	836.740	640.115	836.741
ENTHALPY BTUYLB MOLE H		28.8217	28.8217	28.8216	30.8396	20.8217
ENTROPY. BTU/LB.MOLE-DEG K S	S.H. VAP	S.H. VAP	5.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP
LIQUID FRACTION (L/F) PL	3+H+ TAF	STITE THE	. 54			
COMPOSITION. MOLF FRACTION:		0.750000	0.750000	0.750000	0.750000	0.750000
ORTHO-HYDROGEN X1	0.750000 0.250000	0.250000	0.250000	0.250000	0.250000	0.250000
PARA -HYDROGEN X2	0.250000	. 0*520000	0,000			
	-					
			033(04/01/01)	034(04/01/01)	035(04/01/01)	036(04/01/01)
STREAM NO N-(STYP/KTYP/HTYP)	031(04/01/01)	032(04/01/01)	033(04/01/01/	034104/01/01/	033(04) 01/ 01/	
FLOW+ CFH(NTP) F	635878.	635878.	2143718.	2143718.	8470787.	8470787.
FLOW- LR-MOLEZHR FM	1643.99	1643.99	5542.33	5542.33	21900.2	21900.2
PRESSURF PSIA P	596,000	16.2000	52.0000	52.0000	50.0000	50.0000
TEMPERATURE DEG K	29.5000	20.5200	26.0000	39.2701	39.1735	77.6955
ENTHALPY BTU/LB.MOLE	353.611	353.611	640.115	784.595	784.596	1148.06
ENTROPY. BIUYLB.MOLE-DEG K S	17.5532	20.6125	30.8396	35.2111	35.2904	42.0036
LIQUID FRACTION (L/F) PL	S.C. LIQ	0.697088	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP
COMPOSITION MOLF FRACTION:	3000 614			-	==	
	0.750000	0.750000	0.750000	0.750000	0.750000	0.750000
-	0.250000	0.250000	0.250000	0.250000	0.250000	0.250000
PARA -HYDROGEN XZ	0.230000	4.57400			•	

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STREAM NO N-(STYP/KTYP/HTYP)	037(04/01/01)	038(04/01/01)	039(04/01/01)	040(04/01/01)	041(04/01/01)	042(04/01/01)
	8470787.	8312775.	8312775.	8312775.	-424436.	8737211. 22589.0
FLOW+ CFH(NTP) FLOW+ LB.MOLEZHR FM	21900.2	21491.7	21491.7	21491.7	-1097.33	50.0000
LEGMA CHAMORENCE	47.0000	52.0000	52.0000	50.0000	50.0000	39.1735
PRESSURF + PSIA	77.6489	26.0000	39.2701	39.1735	39.1735	784.596
TEMPERATURE. DEG K	1148.06	640.115	784.595	784.596	784.596	35.2904
ENTHALPY+ BTU/LB MOLE H	42.2121	30.8396	35.2111	35.2904	35.2904	
EMINORIA MIONEDAMORE PRO	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	5.H. VAP
LIQUID FRACTION (L/F) PL	SAMA TAF	36.7.				0.750000
COMPOSITION. MOLE FRACTION:	0.750000	0.750000	0.750000	0.750000	0.750000	
ORTHO-HYDROGEN X1	0.250000	0.250000	0.250000	0.250000	0.250000	0.250000
PARA -HYDROGEN X2	44520000		-			
7		4				
					•	
6			045(04/01/01)	046(04/01/01)	047(04/01/01)	048(04/01/01)
STREAM NO. + N-(STYP/KTYP/HTYP)		044(04/01/01)	045104/01/01/			
• -		0777711	17207984.	17207984.	. 2772125.	1724758.
FLOW+ CFH(NTP) F	8737211.	8737211.	44489.2	44489.2	7167.00	4459.16
FLOW+ LR+MOLE/HP FM	22589.0	22589.0	47.0000	47.0000	600.000	600.000
PRESSURF PSIA	50.0000	47.0000	77.6018	300.000	85.5000	85.5000
TEMPERATURE. DEG K T	77.6027	77.5561	1147.62	3659.43	1160.32	1160.32
ENTHALPY , RTU/LB . MOLE H	1147.20	1147.20		57.0000	33.3969	33.3969
ENTROPY. HTU/LB.MOLE-DEG K S	41.9915	42.2000	42,2060	S.H. VAP	S.H. VAP	S.H. VAP
LIQUID FRACTION (L/F) PL	S.H. VAP	S.H. VAP	S.H. VAP	36116 VAF		
COMPOSITION, MOLE FRACTION:				0.750001	0.750000	0.750000
ORTHO-HYDROGEN X1	0.750000	0.750000	0.750001	0.250000	0.250000	0.250000
PARA -HYDROGEN XZ	0.250000	0.250000	0.250000	4.250000	4120000	
PANA III DAVOCA	** ***			÷	-	
• .				•		
				AE 3/04/01/01\	053(04/01/01)	054(04/01/01)
STREAM NO N-(STYP/KTYP/HTYP)	049(04/01/01)	050(04/01/01)	051(04/01/01)	052(04/01/01)	0331047017017	
SINCHIA MOST IN COLUMN				1047367.	1683244.	1683244.
FLOW. CFH(NTP) F	1047367.	1047367.	104/36/	2707.84	4351.83	4351.83
FLOW, LR.MOLE/HR FM	2707.84	2707.84	2707.84	16.2000	16.2000	16.2000
PRESSURF PSIA	600.000	598.500	598.500	-		20.5200
TEMPERATURE+ DEG K T	85.5000	85,4874	33,2953	20.5200		621.284
ENTHALPY ATUVLB MOLE	1160.32	1160.32	399.808	399.807	20 41/5	33.6873
ENTHALPY HIDEBAMOLE	33.3969	33,4050	19.0180	22.8690		SAT. VAP
EMINOLIS DIOSESS. CARE ALL	S.H. VAP	S.H. VAP	S.C. LIG	0.576780	0.622232	JAIT TOP, J
	weste ear		*:	· ==	A 3EAAA	0.750000
COMPOSITION - MOLE FRACTION:	0.750000	0.750000	0.750000	0.750000		0.250000
ORTHO-HYDROGEN X1		0.250000	0.250000	0.250000	0.250000	0.650000
PARA -HYDROGEN X2	44530000		-			

PARA -HYDROGEN

ORIGINAL PAGE IS OF POOR QUALITY

UNION CARBIDE CORPORATION DATE 11/05/1974

- N2 LIQUEFIER/REFRIGERATOR FOR H2_LIQUEFIER - NASA FUELS STUDY

PAGE 23

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-				1066 7	and the second	The second secon	
*** SEQ = 93 *** BEGI	N .PR	INI	N ₂ LIQUEFIER	/REFRIGERATOR 1	EOR H ₂ LIQUEFI	TER	
STREAM NO N-(STYP/KTYP/HTY	P)	001(01/01/01)	002(01/01/01)	003(01/01/01)	004(01/01/01)	005(01/01/01)	006(01/01/01)
FLOW+ CFHINTP)	F.	13856555.	13856555.	12708755.	5223775.	5223775.	7484980.
	FM	35824.5	35824.5	32857.0	13505.5	13505.5	19351.5
PRESSURF + PSIA	P	407.519	485.331	600.000	600.000	88.0000	600.000
EMPERATURE DEG K	Ť	308.000	308.000	308.000	235.000	147.536	235.000
NTHALPY+ RTU/LB MOLE	.	5605.02	5593.21	5576.10	4582.21	3598.54	4582.21
	- '!. S	41.5135	40.8519	40.0398	36,3516	37.6858	36.3516
	PL	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP
TROGEN	XI	1.000000	1.000000	1,000000	1.000000	1.000000	1.000000
- 1		· · · · · · · · · · · · · · · · · · ·					<u></u>
TREAM NO N- (STYP/KTYP/HTY	P)	007(01/01/01)	008(01/01/01)	009(01/01/01)	010(01/01/01)	011(01/01/01)	015(01/01/01)
LOW+ CFH(NTP)	F	7484980.	9098965.	9098965.	1147800.	1147800.	1147800.
	FM	19351.5	23524.3	23524.3	2967.50	2967.50	2967.50
RESSURE + PSIA	P	600.000	88.0000	88.0000	600.000	600.000	600.000
EMPERATURE: DEG K	т	162.416	148.413	232.000	235.000	162.416	140.000
NTHALPY + RTU/LB.MOLE	н	3441.92	3610.22	4692.08	4582.21	3441.92	2909.88
NTROPY. ATU/LB.MOLE-DEG K	'S'	30.4970	37.7648	43-5560	36.3516	30.4970	26.9483
IQUID FRACTION (L/F)	PL	S.H. VAP	S.H. VAP	S.H. VAP	5.H. VAP	S.H. VAP	S.H. VAP
OMPOSITION MOLE FRACTION:		Jelle 4Mr	20110 101	+			•
	X1	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
TREAM NO N-(STYP/KTYP/HT)	(P)	013(01/01/01)	014(01/01/01)	015(01/01/01)	01=(01/01/01)	017(01/01/01)	018(01/01/01)
				3875190.	3875190.	1147800.	1147800.
LOW+ CFH(NTP)	F	1147800.	3875190.	10018.9	10018.9	2967.50	2967.50
OW. LR.MOLE/HR	FM	2967.50	10018.9	90.0000	88.0000	400.000	400.000
RESSURE + PSIA	P	600.000	90,0000	138.000	149.597	100.223	100.223
EMPERATURE, DEG K	T	99.0000	97.0000		3625.97	946.631	946.631
THALPY, BTU/LB.MOLE	. H	919,675	2879.48	3468.97	37.8705	11.2848	11.2848
NTROPY. RTU/LB.MOLE-DEG K	5	10.7782	31.6080	36.7009		5.C. LIQ	SAT. LIQ
IQUID FRACTION (L/F) OMPOSITION: MOLF FRACTION:	PL	S.C. LIQ	S.H. VAP	S.H. VAP	S.H. VAP		
ITROGEN	X1	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000

			lanuraturo distributi atalia. 11. a. v.	manada e e e e e e e e e e e e e e e e e e	OF POOR	ORIGINAL	
ON CARRIDE CORPORATION	<u> </u>	·	PROBE/370	"(VERSION 03 AUG			DATE 11/05/1974
		410 1 TOUE 5 TED N. A.		•	_	PAG	PAGE 24
NZ LIQUEFIER/REFRIGERATO	 	HS LIGOFFIER - NA	SA FUELS STUUT		ALIT	<u>R</u>	TAGE LEV
STREAM NO N-(STYP/KTYP/H	TYP)	019(01/01/01)	020(01/01/01)	021(01/01/01)	055(01/01/01)	023(01/01/01)	025(01/01/01)
FLOW. CFH(NTP)	F	0.0	3609790.	3609790.	7484980.	0.0	12708755.
FLOW. LP.MOLE/HR	FM	0.0	9332.69	9332.69	19351.5	0.0	32857.0
PRESSURF + PSTA	P	400.000	90.0000		90.0000	90.0000	600.000
TEMPERATURE. DEG K	. T	100.223	97.0000	97.0000	97.0000	63.1366	235.000
ENTHALPY. BTU/LB.MOLE	H	0.0	2879.48	2879.48	2879.48	-0.390625E-02	4582.20
_ENTROPY. BTU/LB.MOLE-DEG K	S	0.0	31.60HO	31.6080	31.6080	-0.107605	36.3516
LIQUID FRACTION (L/F)	PL	SAT. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.C. LIQ	S.H. VAP
COMPOSITION, MOLE FWACTION NITROGEN	; Xl	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
		,					
STREAM NO N-(STYP/KTYP/H	TYP)	026(01/01/01)	027(01/01/01)	028(01/01/01)	029(01/01/01)	030(01/01/01)	031(01/01/01)
"FLOW+ CFH(NTP)	· F	12708755.	1147800.	1147800.	9098965.	13856555.	13856555.
FLOW. LR.MOLE/HR	FM	. 32857.0	2967.50	2967.50	23524.3	35824.5	35824.5
PRESSURF . PSIA	Р	600.000	600.000	600.000	86.0000	600.000	84.0000
TEMPERATURE. DEG K	Ţ	264.051	308.000	264.051	303.000	308.000	305-613
ENTHALPY. RTU/L8.MOLE	н	4985.43	5576.10	4985.43	5592.18	5576.10	5587.63
ENTROPY. BTU/LB.MULE-DEG K	5	37.9699	40.0398	37.9699	47.0233	40.0398	47.0923
LIQUID FRACTION (L/F) COMPOSITION. MOLE FRACTION	PL:	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP
NITHOGEN	X1	1.000000	1.000000	1.000000	1.000000	1.000000	1.000000
			· · · · · · · · · · · · · · · · · · ·	A.E		· 	
STREAM NO N- (STYP/KTYP/H	TYP)	032(01/01/01)	033(01/01/01)	034(01/01/01)	035(01/01/01)		
FLOW+ CFH(NTP)	F	3609790.	10246765.	1147800.	1147800.		
FLOW+ LR.MOLE/HR	FM	9332.69	26491.8	2967.50	2967.50		
PRESSURF + PSIA	P	84.0000	86,0000	86.0000	14.7000		
TEMPERATURE. DEG K	Τ.	300.000	303.560	308.000	300.000		
ENTHALPY. RTU/LB.MOLE	н	5554.64	5599.25	5655.30	5566.48		
ENTROPY. BTU/LB.MOLE-DEG K	S	46.9828	47.0467	47.2300	53.2496		
LIQUID FRACTION (L/F) COMPOSITION, MOLF FRACTION	PL:	S.H. VAP	S.H. VAP	S.H. VAP	S.H. VAP		
NITROGEN	X1, ,	1.000000	1.000000	1,000000	1.000000	Lagrangia para dan anaka kata Paga Paga	
7	m^3/s	$=7.8667 \times 10^{-6}$	(CFH(NTP))	Joules/mole	= 2.324 (BTU/I	B MOLE)	
	Gm n	nole/s = 0.1260	(LB MOLE/HR)	Joules/mole	K = 2.324 (B)	TU/LB MOLE-D	EG K)
	Kilop	ascals = 6.8947	6 (PSIA)	•	-		

ASSUMED PROCESS CONDITIONS

FOR PARAMETIC STUDY

250 TPD H2 LIQUEFIER

LIQUID H ₂	PRODUC'CAPACIT		4,000,000 SC 250 TONS/DAY		
	TEM PERA PRESSUR PARA CO	E	20.57°K 120 PSIG 97 %		
H ₂ FEED PF	RESSURE				14.7 PSIA
H ₂ LIQUEF	ER FEED	PRESSURE			600 PSIA
H2 LIQUEF	IER RECY	CLE PRESSURE			42 PSIA
H ₂ LIQUEF	IER REFRI	GERATION LEVI	EL		26°K
H ₂ TURBIN	E EFFICIE	ENCIES			79%
N2 TURBIN	E EFFICIE	ENCIES			84%
COMPRESS	OR EFFIC H ₂ RECY H ₂ FLASI H ₂ FEED N ₂ RECY N ₂ MAKE N ₂ BOOS	CLE CLE CUP			80% 80% 80% 80% 75% 65%
WARM ENI) APPROA	СН	•		
X-:	1, X-8				8.0 °K
X-3	3, XC-3				3.5 °K
COLD END	APPROAG	СН			
X-2	2, XC-2				0.2 °K
	=	7.8667 x 10 ⁻⁶ 0.0105 (TONS 6.89476(PSIA)	(SCFH) /DAY)	70	

TABLE 6
THEORETICAL AND ACTUAL WORK
OF PARTIAL ORTHO-PARA CONVERSION

COMPOSITION	WORK OF CONVERSION, KWH/LB		
%pH ₂	THEORETICAL	ACTUAL (CORRECTED)*	EFF. %
97.0	1.772	5.018	35.3
79.4	1.670	4.618	36.2
45.5	1.572	4.252	37.0

* CORRECTED TO INCLUDE EFFECT OF PRODUCT FLASHOFF.

TABLE 7 PROCESS REQUIREMENTS FOR PRODUCING REFRIGERATION AT 80 °K LEVEL

REFERENCE: FIGURE 18

	EXPANDER		NITRO	GEN
STR. NO.	FLOW <u>MCFH</u>	TEMP。 <u> </u>	FLOW <u>MCFH</u>	TEMP• K
2 4	3,659 62,142	308.0 308.0	3,659 27,450	308.0 308.0
5	27,450	85.5	27,450	85.5
11	4,000	81.2	4,000	80.9
21	25,683	81.2	25,683	81.2
45	24,742	77. 5	24 , 742	77.5
46	59,433	299.6	24,742	299.6
49	1,426	85.5	1,426	85.5
56	2,368	71.4	2,368	71.4
57	2,368	300.0	2,368	300.0
60	61,801	300.6	2 7,1 10	300.7
70	34,692	128.6	•	
71	34,692	77.0		

POWER REQUIREMENTS

	PRESSURE-PSIA		POWER	-BHP
MACHINE	SUCTION	DISCHARGE	EXPANDER	NITROGEN
RECYCLE COMPRESSOR (P-RC)	42	300	193,235	85,800
SUBCOOLING FLUID COMPR (P-SCF)	15	.42	3,731	3,731
FEED COMPRESSOR	14.7	300	19,776	19,776
N ₂ LIQUEFIER			0	36,586
EXPANDER CREDIT (E-3)	300	50	(18,070)	0
EXPANDER CREDIT (E-1 & E-2)			(5,198)	(5,198)
	NE	T	193,474	140,695
	UNIT WO	ORK, KWH/LB	6.92	5.03

 m^3/s

= 7.8667 x 10⁻³ (MCFH) = 6.89476 (PSIA) = 0.7457 (BHP) = 7.9367 (KWH/LB) KILOPASCALS KW KILOJOULE/GM

TABLE 8 POWER REQUIREMENTS PARAMETRIC STUDY BASE CASE

COMPRESSORS	<u>BHP</u>
HYDROGEN RECYCLE (P-RC)	78,755
HYDROGEN SUBCOOLING FLUID (P-SCF)	2,893
HYDROGEN FEED	23,675
NITROGEN RECYCLE (P-3)	29,517
NITROGEN FEED (P-4)	2,502
SUB TOTAL	137,342
FORECOOLER FOR N ₂ REFRIGERATOR N ₂ REFRIGERATOR ADDITIONS	3,857 <u>686</u>
SUB TOTAL	141,885
HYDROGEN TURBINE NO. 1 (E-1)	(2,253)
HYDROGEN TURBINE NO. 2 (E-2)	(2,088)
TOTAL	137,544

 $137,544 \times 0.7457 = 102610 \text{ KW}$ $4,000,000 \text{ SCFH } \times .00521213 \text{ lb/ft}^3 = 20848.5 \text{ lb/hr}$

$$\frac{102610}{20848.5}$$
 = 4.9217 KWH/LB

KW = 0.7457 (BHP) $m^3/s = 7.8667 \times 10^{-6} \text{ (SCFH)}$ $Kg/m^3 = 16.0185 \text{ (LB/FT}^3)$ $Kg/s = 1.26 \times 10^{-4} \text{ (LB/HR)}$ KILOJOULES/GM = 7.9367 (KWH/LB)

TABLE 9
THERMODYNAMIC LOSSES
FOR HYDROGEN LIQUEFIER

HEAT EXCHANGERS		KWH/LB H ₂		<u>%</u>
X-1 X-2 X-3 X-4 X-6 X-7 X-8	TOTAL	0.0967 0.0071 0.1422 0.0245 0.0390 0.0480 0.0414	0.3989	19.06
CONVERTERS XC-2 XC-3 XC-4 XC-5	TOTAL	0.0249 0.0593 0.0444 0.00001	0.1286	6.15
THROTTLING VALVES V-1 V-3 V-4 V-5	TOTAL	0.0645 0.0212 0.0440 0.0123	0.1420	6.79
MIXING	TOTAL		0.0514	2.46
HEAT LEAK	TOTAL	GITD MOURI	0.0360 0.7569	1.72 36.17
COMPRESSORS P-RC P-SCF		0.8929 0.0323	0.9252	44.22
TURBINES E-1 E-2	TOTAL	0.1786 0.2299	0.4085 0.0019	19.52 0.09
MISCELLANEOUS		TOTAL LOSSES	2.0925	100.00
KILOJOULES/GM =	7.9367 (KWH)	/LB) 84	-	

TABLE 10

THERMODYNAMIC LOSSES
FOR NITROGEN REFRIGERATOR

HEAT EXCHANGERS X-1 X-2 X-3		KWH/LB H ₂ 0.0200 0.0141 0.0274	<u>2</u>	<u>%</u>
x -4		0.0132	0.0747	9.47
FORECOOLER_			0.0866	10.98
THROTTLING VALVES			0.0022	0.28
MIXING			0.0079	1.00
HEAT LEAK			0.0034	0.43
COMPRESSORS				
P-1 P-2 P-3 P-4	TOTAL	0.0669 0.0505 0.3182 0.0313	0.4669	59.19
TURBINES				
E-1 E-2	TOTAL	0.0698 <u>0.0773</u>	0.1471	18.65
	TOTAL		0.7888	100.00

TABLE 11
SUMMARY OF OVERALL
THERMODYNAMIC LOSSES

BY PROCESS	KWH/LB H ₂	%
H ₂ LIQUEFIER	2.0925	66.37
N ₂ REFRIGERATOR	0.7888	25.02
FEED COMPRESSOR	0.2713	8.61
TOTAL LOSSES	3.1526	100.00
THEORETICAL WORK	1.7728	
ACTUAL WORK	4.9254	
BY EQUIPMENT TYPE		
COMPRESSORS TURBINES HEAT EXCHANGERS CONVERTERS FORECOOLER THROTTLING MIXING HEAT LEAK & MISCELLANEOUS	1.6634 0.5556 0.4736 0.1286 0.0866 0.1442 0.0593 0.0413	52.76 17.63 15.02 4.08 2.75 4.57 1.88 1.31
TOTAL	3.1526	100.00

THERMODYNAMIC EFFICIENCY = $\frac{1.7728}{4.9254}$ x 100 = 36.0%



PROCESS BASIS FOR ACTUAL BASE CASE 2500 TPD LIQUID HYDROGEN

- Plant capacity = 40,000,000 SCFH (2501.8 TPD) liquid hydrogen product at 14.7 psia and 20.23 °K.
- Feedstock delivered to battery limits at 214.7 psia, 95 °F and with the following composition:

H ₂	96.6
N_2	1.2
CO	1.2 0.3
CO ₂	
CH ₄	$\frac{0.7}{100.0}$

- 3. Plant consists of 10 process modules, in parallel, with product capacity of 4,000,000 SCFH per module.
- 4. Electric motors for prime movers for all compressors and pumps.
- Combined motor efficiency and gear loss allowance of 93.5% to 98.4% depending upon speed and power rating.
- 6. On stream time is 95%.
- 7. Leakage and other losses as presented in Table 27.
- 8. Other liquefier and refrigerator process conditions as given for Idealized Base Case, Tables 3 and 4 .
- 9. Cryogenic absorption purifier used for final purification of ${\rm H}_2$.
- 10. Liquefaction complex arrangement as per block flow diagram, Figure 19.
- 11. Assumes technology available in 1974.
- 12. Composition = 97% para hydrogen.
- 13. Work output recovered from hydrogen turbines via electric generators.
- 14. Standard Cubic Foot basis = 14.7 psia and 70° F

$$m^3/s = 7.8667 \times 10^{-6}$$
 (SCFH)
 $Kg/s = 0.0105$ (TPD)
 $Kilopascals = 6.89476$ (psia)
 $^{\circ}K = (^{\circ}F-32)/1.8 + 273.15$

UTILITY SUMMARY HYDROGEN LIQUEFACTION COMPLEX 2500 TONS/DAY LIQUID HYDROGEN

ACTUAL BASE CASE (1974)

ELECTRICAL POWER

### HYDROGEN COMPRESSORS 836,990 634,630 NITROGEN RECYCLE COMPRESSOR 340,920 262,200 FORECOOLER 42,130 33,100 AIR COMPRESSOR, N, PLANT 20,000 15,950 PURIFIER HEAT PUMP COMPRESSOR 42,550 33,430 HYDROGEN FEED/BOOSTER COMPRESSOR 72,440 56,300 NITROGEN FEED COMPRESSOR 34,000 26,710 HYDROGEN FEED COMPRESSOR 34,000 26,710 HYDROGEN DRIER 1,050 7,260 PUMPS 2040 1,810 HYDROGEN TURBINE RETURN -44,500 -31,550 NET SUB TOTAL 1,347,620 1,039,840 ### PRODUCTION AUXILIARIES COOLING TOWER AND WATER SUPPLY 58,000 49,520 PLANT AIR COMPRESSOR AND DRIER 4,750 3,140 PURGE BLOWER AND THAW HEATER 4,750 13,430 MISCELLANEOUS 950 17,860 PROCESS CONTINGENCY (5%) 70,800 56,190 SUB TOTAL 1,486,870 1,179,980 #### PLANT AUXILIARIES ROAD AND EXTERIOR LIGHTING 500 BUILDING LIGHTING, HEATING, AIR COND. CRANES 2,200 **TOTAL, ELECTRICAL POWER 1,182,180 WATER				
NITROGEN RECYCLE COMPRESSOR 340,920 262,200 FORECOOLER 42,130 33,100 AIR COMPRESSOR, N, PLANT 20,000 15,950 PURIFIER HEAT PUMP COMPRESSOR 42,550 33,430 HYDROGEN FEED/BOOSTER COMPRESSOR 72,440 56,300 NITROGEN FEED COMPRESSOR 34,000 26,710 HYDROGEN FEED COMPRESSOR 1,050 7,260 PUMPS 1,050 7,260 PUMPS 2,040 1,810 HYDROGEN TURBINE RETURN -44,500 -31,550 NET SUB TOTAL 1,347,620 1,039,840 PRODUCTION AUXILIARIES COOLING TOWER AND WATER SUPPLY 58,000 49,520 PLANT AIR COMPRESSOR AND DRIER 4,750 3,140 PURGE BLOWER AND THAW HEATER 4,750 13,430 MISCELLANEOUS SUB TOTAL 66,450 83,950 PROCESS CONTINGENCY (5%) 70,800 56,190 SUB TOTAL 1,486,870 1,179,980 PLANT AUXILIARIES ROAD AND EXTERIOR LIGHTING BUILDING LIGHTING, HEATING, AIR COND. 2,200 TOTAL, ELECTRICAL POWER .1,182,180	PRODUCTION		BHP	<u>KW</u>
## PRODUCTION AUXILIARIES COOLING TOWER AND WATER SUPPLY 58,000 49,520 91ANT AIR COMPRESSOR AND DRIER 4,750 3,140 9URGE BLOWER AND THAW HEATER 4,750 13,430 MISCELLANEOUS 950 17,860 83,950 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,860 950 17,800 56,190 950 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,800 950 17,80	NITROGEN RECYCLE COM FORECOOLER AIR COMPRESSOR, N, PLA PURIFIER HEAT PUMP CO HYDROGEN FEED/BOOSTE NITROGEN FEED COMPRES HYDROGEN DRIER PUMPS HYDROGEN TURBINE RETU	PRESSOR ANT MPRESSOR R COMPRESSOR SSOR SUB TOTAL	340,920 42,130 20,000 42,550 72,440 34,000 1,050 2,040 1,392,120 -44,500	262,200 33,100 15,950 33,430 56,300 26,710 7,260 1,810 1,071,390 -31,550
COOLING TOWER AND WATER SUPPLY 58,000 49,520 PIANT AIR COMPRESSOR AND DRIER 4,750 3,140 PURGE BLOWER AND THAW HEATER 4,750 13,430 MISCELLANEOUS 950 17,860 SUB TOTAL 68,450 83,950 PROCESS CONTINGENCY (5%) 70,800 56,190 SUB TOTAL 1,486,870 1,179,980 PLANT AUXILIARIES ROAD AND EXTERIOR LIGHTING BUILDING LIGHTING, HEATING, AIR COND. 1,300 CRANES 500 TOTAL, ELECTRICAL POWER .1,182,180		SOR TOTAL	1,347,020	1,033,040
PLANT AIR COMPRESSOR AND DRIER 4,750 3,140 PURGE BLOWER AND THAW HEATER 4,750 13,430 MISCELLANEOUS 950 17,860 SUB TOTAL 68,450 83,950 PROCESS CONTINGENCY (5%) 70,800 56,190 SUB TOTAL 1,486,870 1,179,980 PLANT AUXILIARIES ROAD AND EXTERIOR LIGHTING BUILDING LIGHTING, HEATING, AIR COND. 1,300 CRANES 500 TOTAL, ELECTRICAL POWER .1,182,180				40.500
SUB TOTAL 1,486,870 1,179,980 PLANT AUXILIARIES ROAD AND EXTERIOR LIGHTING BUILDING LIGHTING, HEATING, AIR COND. CRANES TOTAL, ELECTRICAL POWER .1,182,180	PLANT AIR COMPRESSOR A PURGE BLOWER AND THAY MISCELLANEOUS	AND DRIER W HEATER SUB TOTAL	4,750 4,750 950 68,450	3,140 13,430 17,860 83,950
PLANT AUXILIARIES ROAD AND EXTERIOR LIGHTING BUILDING LIGHTING, HEATING, AIR COND. CRANES TOTAL, ELECTRICAL POWER 1,300 400 2,200	PROCESS CONTINGENCY			<u> </u>
ROAD AND EXTERIOR LIGHTING BUILDING LIGHTING, HEATING, AIR COND. CRANES TOTAL, ELECTRICAL POWER 1,300 400 2,200		SUB TOTAL	1,486,870	1,1/9,980
BUILDING LIGHTING, HEATING, AIR COND. CRANES 1,300 400 2,200 TOTAL, ELECTRICAL POWER .1,182,180	PLANT AUXILIARIES			
1011111 Indiana in the second of the second	BUILDING LIGHTING, HE	HTING LATING, AIR CON	D .	1,300 400
WATER	TC	.1,182,180		
	WATER			
COOLING WATER MAKEUP - GPM 42,000		P - GPM		42,000

88

Cont'd....

TABLE 13 - CONT'D

CHEMICALS

SULFURIC ACID FOR WATER TREATMENT, LB/HR 4,000 DESSICANTS AND ADSORBENTS, LB/YR 450,000

ANNUAL THAW

 N_2 FOR PLANT PURGE AND THAW 68,000,000 CF. HEATING FUEL 2×10^9 BTU

Kg/s = 0.0105 (TONS/DAY) KWH = 0.7457 (BHP) m^3/s = 6.3089 x 10^{-5} (GPM) Kg/s = 1.260 x 10^{-4} (LB/HR) Kg/s = 1.4383 x 10^{-8} (LB/YR) m^3 = 0.02832 (CF) KILOJOULES = 1.05435 (BTU)

TABLE 14

ABSORPTION VS ADSORPTION PROCESSES HYDROGEN PURIFICATION 250 TPD PURIFIER MODULE

	<u>ABSORPTION</u>	<u>ADSORPTION</u>
INVESTMENT	\$3,3000,000	\$4,300,000
UTILITIES		
LIQUID NITROGEN, CFH	281,000	345,000
STEAM, LB/HR		5,000
COOLING WATER, GPM	1,500	1,500
ELECTRICAL ENERGY, KW		
FEED COMPRESSOR ALLOCATION	214	600
RECIRCULATION COMPRESSOR		410
HEAT PUMP COMPRESSOR	3,343	
PUMPS	181	
FOR LIQUID N ₂	2,861	5,039
TOTAL	6,599	6,049
HYDROGEN LOSS, CFH	270,000	290,000

$$m^3/s$$
 = 7.8667 x 10⁻⁶ (CFH)
Kg/s =1.260 x 10⁻⁴ (LB/HR)
 m^3/s = 6.3089 x 10⁻⁵ (GPM)



TABLE 15 THERMAL EFFICIENCY LIQUID H₂ VIA COAL GASIFICATION

FEEDSTOCK GASIFIER

Input: 769 ST/hr coal at 12,500 Btu/lb.

323,600 BHP Mechanical Energy

67,800 KW Electrical Energy

4,770 MM Btu/hr from Fuel Gas

Output: 47.69 MMSCFH H2 Feedstock at 308 Btu/SCF

POWER GASIFIER

Input: 1195 ST/hr coal at 12,500 Btu/lb

397,700 BHP Mechanical Energy

59,300 KW Electrical Energy

Output: 76.81 MMSCFH Fuel Gas at 292 Btu/SCF

H₂ LIQUEFIER

Input: 47.69 MMSCFH H₂ Feedstock at 308 Btu/SCF

1,182,180 KW Electrical Energy

Output: 40.00 MMSCFH Liquid H2 at 318.5 Btu/SCF

2.675 MMSCFH Tail Gas at 209 Btu/SCF

ENERGY CONVERSION

Input: 60.48 MMSCFH Fuel Gas at 292 Btu/SCF

Output: 721,400 BHP Mechanical Energy

1,309,300 KW Electrical Energy

Note: All heating values are HHV basis

THERMAL EFFICIENCIES	MMB	THERMAL	
· · · · · · · · · · · · · · · · · · ·	INPUT	OUTPUT	EFF%
Feedstock Gasifier	25,050	14,690	58.6
Power Gasifier	31,080	22,430	72.2
H ₂ Liquefier	18,730	13,300	71.0
Energy Conversion	17,660 .	6,303	35.7
Overall	48,540	12,740	26.2

TABLE 15 (CONT'D)

Kg/s = 0.25120 (ST/HR)
Joules/gm = 2.324 (Btu/lb)
KW = 0.7457 (BHP)
KW = 292.88 (MM Btu/hr)
m³/s = 7.8667 (MMSCFH)
Kilojoules/m³ = 37.230 (Btu/SCF)

TABLE 16 THERMAL EFFICIENCY LIQUEFIED NATURAL GAS

SNG VIA LURGI PROCESS (8)

Coal to Plant:

25,947 ST/D at HHV = 8872 Btu/lb

Gaseous SNG, at 900 psig:

256.6 MMSCFD at HHV = 972 Btu/SCF

Heat in

Heat III	Coal	To gasifier To boiler	M 1b/hr 1722 440 2162	MM Btu/hr 15,280 3,900 19,180
Heat out	ţ			
	SNG		469.6	10,391
	Tar		89.5	1,387
	Tar oil	[36.9	572
	Naphti		18.4	318
	Pheno		8.7	122
	Ammor		16.9	141
	Sulfur		12.3	40

Thermal Eff. (SNG) = $\frac{10,391}{19,180-1,387-572-318}$ x 100 = 61.47%

LIQUEFACTION PLANT (9, 10)

Feedstock:

99⁺% CH₄ at 650 psig & 60 °F

Product:

173 MMCFD LNG

Power:

63,840 KW

ENERGY IN:	<u>MMCFD</u>	MM BTU/HR
SNG - Feedstock	173	7006.5
Power	19.11	774.0
Credit (pipe pressure)	(0.77)	(31.2)
Net	191.34	7749.3



TABLE 16 (CONT'D.)

ENERGY OUT

MMCFD

MM BTU/HR

LNG

173

7006.5

Thermal Efficiency (LNG) = $\frac{7006.5}{7749.3}$ x 100 = 90.41%

OVERALL PROCESS

For 173 MMCFD of LNG

SNG Required = 191.34 MMCFD

Coal Required = 1612 M lb/hr,

14303 MM Btu/hr

Fuel By-products

1698 MM Btu/hr

Efficiency, overall process = $\frac{7006.5}{14303 - 1698} \times 100 = 55.6\%$

Kg/s = 0.01050 (ST/D) Kilojoules/Kg = 2.324 (Btu/lb) $Kilojoules/m^3 = 37.230 (Btu/SCF)$ Kilopascals = 6.89476 (psig + 14.7) Kg/s = 0.1260 (M lb/hr) Kw = 292.88 (MM Btu/hr) $^{\circ}K = (^{\circ}F - 32)/1.8 + 273.15$ $m^3/s = 0.32778 (MMCFD)$

THERMAL EFFICIENCY

METHANOL

PRODUCT RATE:

800 TONS/DAY METHANOL

PROCESS:

HIGH PRESSURE SYNTHESIS WITH

SYNTHESIS GAS VIA STEAM REFORMING OF

NATURAL GAS

BASIS:

1 TON METHANOL

NATURAL GAS:

38 MM BTU

ELECTRICITY:

35 KWH

HEAT IN

MMBTU

NATURAL GAS:

38.0

ELECTRICITY: $35 \times 3414 \times 10^{-6}$

0.119

HEAT OUT

METHANOL

2,000 lb at 10,259 Btu/lb \times 10⁻⁶

20.52

THERMAL EFFICIENCY = $\frac{20.52}{38.119}$ x 100 = 53.8%

Kg/s = 0.0105 (TONS/DAY)

Kilojoules = 1.05435×10^6 (MM BTU)

Kq = 907.185 (TON)

Kilojoule = 3600 (KWH)

Kq = 0.45359 (LB)

Kilojoules/Kg = 2.324 (BTU/LB)

LIQUEFACTION COST ACTUAL BASE CASE (1974) DCF FINANCING

BASIS

25 - YEAR PROJECT LIFE 16 - YEAR SUM-OF-THE-YEARS'-DIGITS DEPRECIATION 100% EQUITY CAPITAL 12% DCF RETURN RATE 48% FEDERAL INCOME TAX RATE

I = TOTAL PLANT INVESTMENT	\$ 528,197,000	
S = STARTUP COSTS	14,500,000	
W = WORKING CAPITAL	17,580,000	
N = TOTAL NET OPERATING ANNUAL COST	\$ 29,348,900	
G = ANNUAL LIQUID N ₂ PRODUCTION	$1733.8 \times 10^6 LB/YR$	
a = ESCALATION FACTOR NO ESCALATION	1.00	
aN + 0.2353 I + 0.1275 S + 0.2308 W		
UNIT LIQUEFACTION COST = G		

$$= \frac{1(29.349) + 0.2353(528.197) + 0.1275(14.50) + 0.2308(17.58)}{1733.8}$$

= \$0.09202 PER LB.

$$Kg/s = 1.4383 \times 10^{-8} \text{ (LB/YR)}$$

 $$/Kg = 2.2046 \text{ ($/LB)}$

LIQUEFACTION COST ACTUAL BASE CASE (1974) UTILITY FINANCING

BASIS:

20 YEAR PROJECT LIFE

5% PER YEAR STRAIGHT LINE DEPRECIATION ON TOTAL CAPITAL REQUIREMENT EXCLUDING WORKING CAPITAL

48% FEDERAL INCOME TAX RATE

C = TOTAL CAPITAL REQUIREMENT	\$649,410,000
W = WORKING CAPITAL	17,580,000
N = TOTAL NET OPERATING ANNUAL COST	29,348,900
G = ANNUAL LIQUID H ₂ PRODUCTION	$1733.8 \times 10^6 \text{ LB/YR}$
d = FRACTION DEBT	0.75
i = INTEREST RATE ON DEBT	9%
r = RETURN ON EQUITY	15%
p = RETURN ON RATE BASE	
a = ESCALATION FACTOR - NO ESCALATION	1.00
p = (d) i + (1-d) r	
p = (0.75) 9 + (0.25) 15	
p = 10.5	
an + 0.05 (C-w) + 0.005 [p	$0 + \frac{48}{52} (1-d) r (C+W)$
UNIT LIQUEFACTION COST = G	······································

$$= \frac{1.0 (29.349) + 0.05(631.830) + 0.005 [10.5 + \frac{48}{52} (.25) 15](666.99)}{1733.8}$$

= \$0.06200 PER LB.

 $Kg/s = 1.4383 \times 10^{-8}$ (LB/YR) \$/Kg = 2.2046 (\$/LB)

CAPITAL INVESTMENT LIQUEFACTION COMPLEX ACTUAL BASE CASE - 1974

2500 TPD LIQUID H2

TOTAL PLANT INVESTMENT	\$528,197,000
INTEREST DURING CONSTRUCTION(1)	89,133,000
STARTUP COSTS	14,500,000
WORKING CAPITAL (2)	17,580,000
TOTAL CAPITAL REQUIREME	NT \$649,410,000

- (1) at 9% interest rate on total plant investment for 1.875 years
- (2) Sum of (1) materials and supplies at 0.9% of total plant investment plus (2) net receivables on product hydrogen at 1/24 of annual production at \$3.00/MM BTU.

Kg/s = 0.0105 (TPD) $$/Kilojoule = 9.4845 \times 10^{-7}$ (\$/MM BTU)

TABLE 21

ANNUAL OPERATING COST LIQUEFACTION COMPLEX ACTUAL BASE CASE - 1974

2500 TPD LIQUID H₂

RAW MATERIALS FEEDSTOCK - FROM COAL GASIFIER

CHEMICALS AND ADSORBENTS H ₂ SO ₄ 4,000 LB/HR @ \$50.00/TON	\$	832,000
DESSICANTS & ADSORBENTS 450,000 LB/YR @ 67¢/LB		301,500
UTILITIES		
MAKEUP WATER 15,000 GPM @ 30¢ /M GAL ELECTRICITY - FROM COAL GASIFIER	2	2,247,000
LABOR OPERATING LABOR SUPERVISION	:	1,797,600 230,800
ADMINISTRATION AND OVERHEAD	-	1,217,000
SUPPLIES		
OPERATING (30% OF OPERATING LABOR) MAINTENANCE (1.5% OF INVESTMENT)		540,000 7,923,000
TAXES AND INSURANCE (2.7% of INVESTMENT)	_1	4,260,000
TOTAL OPERATING COST	\$ 2	9,348,900

$$Kg/s = 0.0105 \text{ (TPD)}$$

 $Kg/s = 1.260 \times 10^{-4} \text{ (LB/HR)}$
 $\$/Kg = 1.1023 \times 10^{-3} (\$/TON)$
 $Kg/s = 1.4383 \times 10^{-8} \text{ (LB/YR)}$
 $\rlap/e/Kg = 2.2046 (\rlap/e/LB)$
 $m^3/s = 6.3089 \times 10^{-5} \text{ (GPM)}$
 $\rlap/e/m^3 = 0.26417 (\rlap/e/M GAL)$

TABLE 22

LIQUEFACTION COST

PROJECTED TO 1985-2000 TIME PERIOD

DCF FINANCING

BASIS

Same as per Table 18 except:

I = Total Plant Investment = \$496,500,000 W = Working Capital = \$16,850,000 N = Total Net Operating Annual Cost = \$27,500,000 Cost = 1(27.50) + 0.2353(496.5) + 0.1275(14.5) + 0.2308(16.85)

Unit Cost = $\frac{1(27.50) + 0.2353(496.5) + 0.1275(14.5) + 0.2308(16.85)}{1733.8}$

= \$0.08655 per lb.

UTILITY FINANCING

BASIS

Same as per Table 19 except:

C = Total Capital Requirement = \$611,600,000 W = Working Capital = \$16,850,000 N = Total Net Operating Annual Cost = \$27,500,000 $Unit Cost = 1(27.5) + 0.05(594.75) + 0.005[10.5 + <math>\frac{48}{52}$ (.25) 15](628.45)

= \$0.05831 per lb.

TABLE 23

CAPITAL INVESTMENT

COAL GASIFICATION COMPLEX

2500 TPD LIQUID H_2

•		\$MM
SECTION	1974	1985/2000
H ₂ and Fuel Gas Production Coal Preparation and Water Gas Shift	410.3	368.7
Raw Gas Compression	129.9	
H ₂ and Fuel Gas Purification Sulfur and CO ₂ Removal	110.4	97.8
O2 Plant and Compression	309.2	218.0
Power and Steam Generation	279.1	215.1
Electrical Substation and Switchgear	51.1	47.6
Water Treatment and Cooling	28.3	28.3
General Facility, Roads, Building, Etc.	21.6	18.2
SUB TOTAL PLANT INVESTMENT	1339.9	993.7
PROJECT CONTINGENCY AT 15 PER CENT	200.9	149.1
TOTAL PLANT INVESTMENT	1540.8	1142.8

//

TABLE 24 GASIFICATION COST DCF FINANCING

BASIS:

25 - YEAR PROJECT LIFE

16 YEAR SUM-OF-THE-YEAR'S DIGITS DEPRECIATION

100% EQUITY CAPITAL

12% DCF RATE OF RETURN

48% FEDERAL INCOME TAX RATE

I = TOTAL PLANT INVESTMENT, \$ MM

S = STARTUP COSTS, \$ MM

W = WORKING CAPITAL, \$ MM

N = TOTAL NET OPERATING ANNUAL COST, \$ MM

G = ANNUAL LIQUID H₂ PRODUCTION, 1733.8 MM LB/YR

a = ESCALATION FACTOR = 1.00

UNIT GASIFICATION COST = $\frac{aN + 0.2353 \text{ I} + 0.1275 \text{ S} + 0.2308 \text{ W}}{G}$

YEAR		1974		1985-2000		
COAL COST (1)	0.35	0.50	0.75	0.35	0.50	0.75
I	1540.8	1540.8	1540.8	1142.8	1142.8	1142.8
S	52.7	65.4	86.6	39.9	49.5	65.4
w	39. 6	50. 6	69.0	29.6	37.8	51.6
N	249.2	313.0	419.2	189.0	236.8	316.5
UNIT COST, ¢/LB(2)	36.20	40.12	46.64	27.10	30 •03	34.93

(1) \$/MM BTU

(2) For gasification only. Liquefaction costs must be added.

Kg/s = 0.014383 (MM LB/YR)

 $\frac{10^{-7}}{10^{-7}}$ (\$/MM BTU)

c/Kg = 2.2046 (c/LB)

TABLE 25

GASIFICATION COST UTILITY FINANCING

BASIS:

20-YEAR PROJECT LIFE

5% STRAIGHT LINE DEPRECIATION ON TOTAL CAPITAL INVESTMENT 48% FEDERAL INCOME TAX RATE

C = TOTAL CAPITAL REQUIREMENT, \$MM

W = WORKING CAPITAL, \$ MM

N = TOTAL NET OPERATING ANNUAL COST, \$ MM

G = ANNUAL LIQUID H₂ PRODUCTION = 1733.8 MM LB/YR

d = FRACTION DEBT = 0.75

r = RETURN ON EQUITY = 15%

i = INTEREST RATE ON DEBT = 9%

p = RETURN ON RATE BASE

a = ESCALATION FACTOR = 1.00

$$p = d(i) + (1 - d) r$$

 $p = 10.5$

UNIT GASIFICATION COST = $\frac{8N + 0.05 (C-W) + 0.005 (p + \frac{48}{52} (1-d) r) (C+W)}{G}$

YEAP.		1974			1985/2000	<u></u>
COAL COST (1)	0.35	0.50	0.75	0.35	0.50	0.75
I	1540.8	1540.8	1540.8	1142.8	1142.8	1142.8
S (2)	52.7	65.4	86.6	39.9	49.5	65.4
W	39.6	50.6	69.0	29.6	37.8	51.6
INTEREST (3)	260.0	260.0	260.0	192.8	192.8	192.8
С	1893.1	1916.8	1956.4	1405.1	1422.9	1452.6
N	249.2	313.0	419.2	189.0	236.8	316.5
UNIT COST						
¢/LB (4)	27.50	31.36	37.78	20.64	23.53	28.35

^{(1) \$/}MM BTU

- (2) Sum of (a) raw materials inventory of 60 days at full rate and (b) materials and supplies at 0.9% of total plant investment.
- (3) At 9% interest rate on total plant investment
- (4) For gasification only. Liquefaction costs must be added.

TABLE 25 (CONT'D.)

Kg/s = 0.014383 (MM LB/YR) \$/Kilojoule = 9.4845 x 10^{-7} (\$/MM BTU) $\phi/Kg = 2.2046$ (ϕ/LB)

TABLE 26 TOTAL UNIT COST OF LIQUID $\rm H_2$ VIA COAL GASIFICATION

¢ PER LB

YEAR		1974		1985-2000			
	· 						
Cost of Coal (1)	0.35	0.50	0.75	0.35	0.50	0.75	
UTILITY FINANCING		,					
Gasification	27.50	31.36	37.78	20.64	23.53	28.35	
Lique faction	6.20	6.20	6.20	5.83	5.83	5.83	
Total	33.70	37.56	43.98	26.47	29.36	34.18	
DCF FINANCING							
Gasification	36.20	40.12	46.64	27.10	30.03	34.93	
Liquefaction	9.20	9.20	9.20	8.66	8.66	8.66	
Total	45.40	49.32	55.82	35.76	38.69	43.59	

^{(1) \$/}MM BTU

c/Kg = 2.2046 (c/LB)

 $[\]frac{10^{-7}}{\text{($/MM BTU)}}$

TABLE 27 HYDROGEN PROCESS LOSSES 2500 TPD LIQUID H₂ PRODUCT

LIQUEFIER LOSSES	MSCFH
Product Flash to Storage	995
Equipment and Piping Leakage	1,250
Compressor Leakage	1,665
Expander Leakage	815
Total	4,725
Less: Recovery of Turbine Leakage	735
Storage Losses	290
Total	1,025
Net Loss	3,700
PURIFIER LOSSES	
Equipment Leakage	325
Compressor Leakage	325
Purge	42
Stripping Gas and Solubility Loss	1,194
Total	1,886
Combined Total Losses	5,586
Total H ₂ Feed	45,586
Percentage Loss	12.3%

Kg/s = 0.0105 (TPD) $m^3/s = 7.8667 \times 10^{-3} \text{ (MSCFH)}$

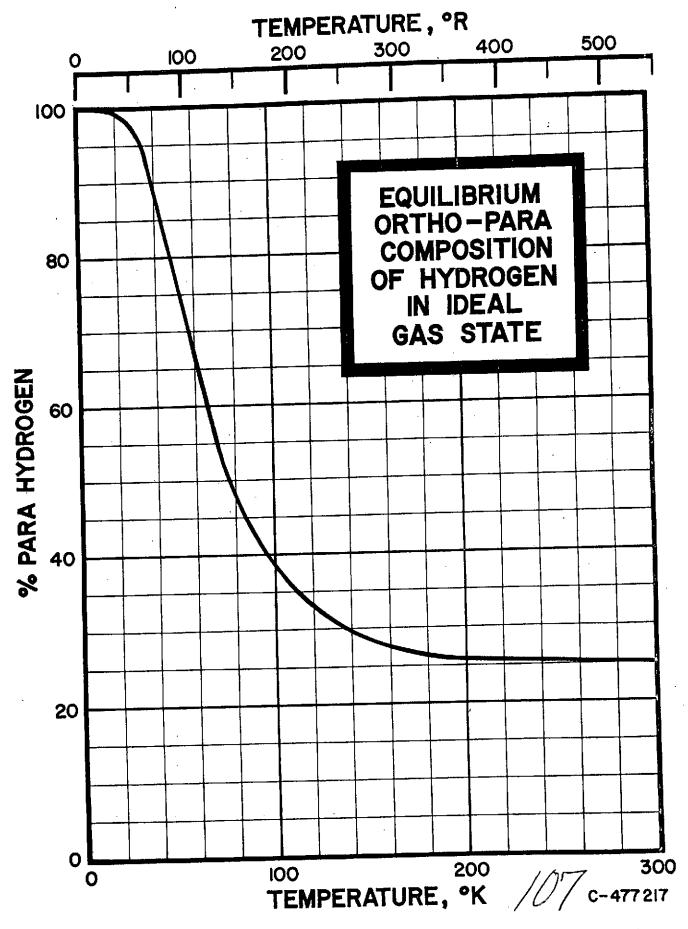
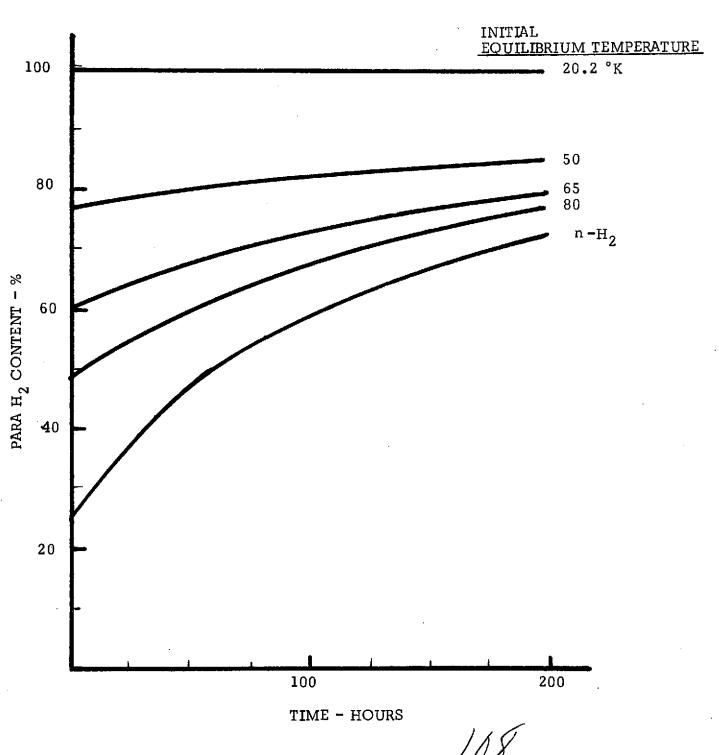
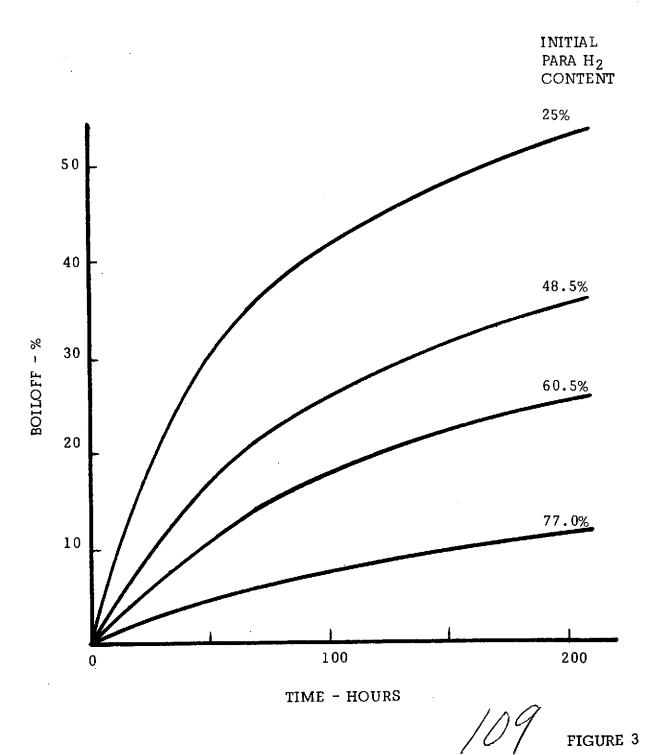


FIGURE 1

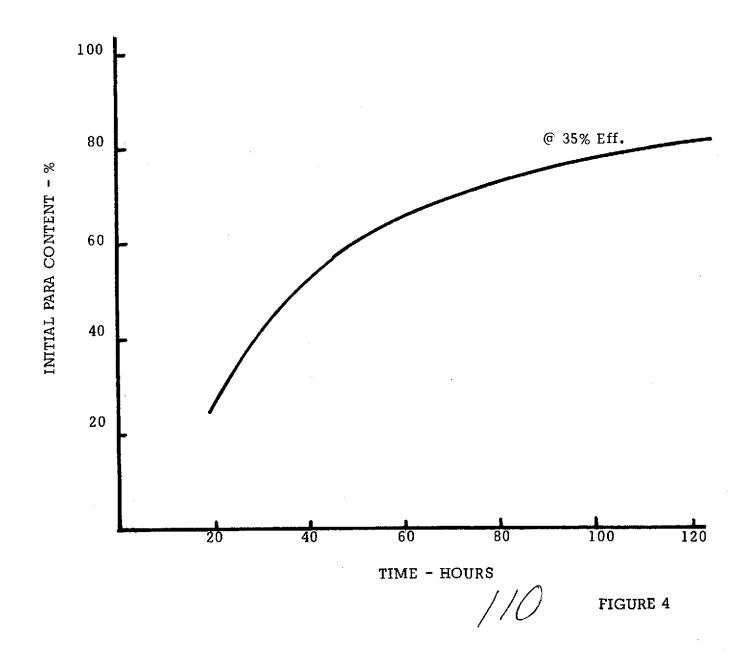
LIQUID H₂ COMPOSITION VS TIME FOR UNCATALYZED ORTHO-PARA CONVERSION



BOILOFF OF LIQUID H_2 AS RESULT OF UNCATALYZED AUTOCONVERSION TO PARA FORM



BREAKEVEN TIME FOR PARTIALLY CONVERTED LIQUID H₂

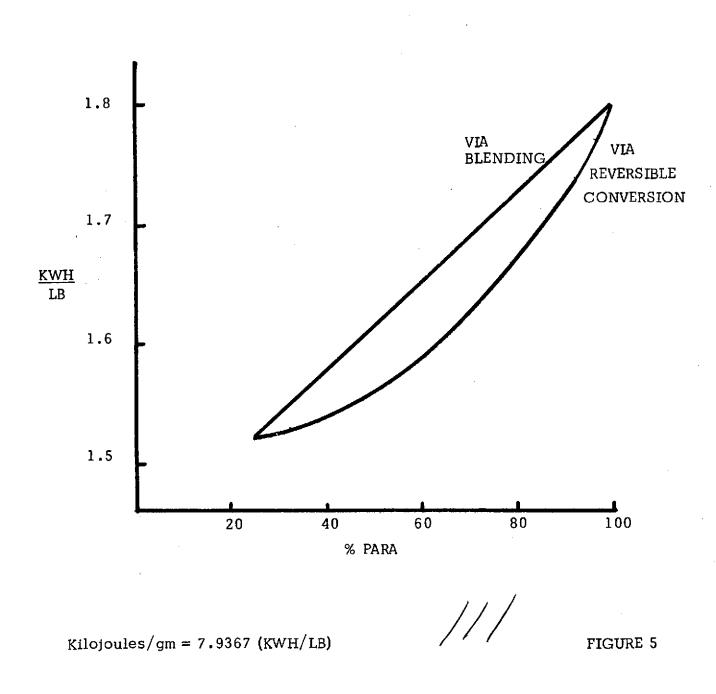


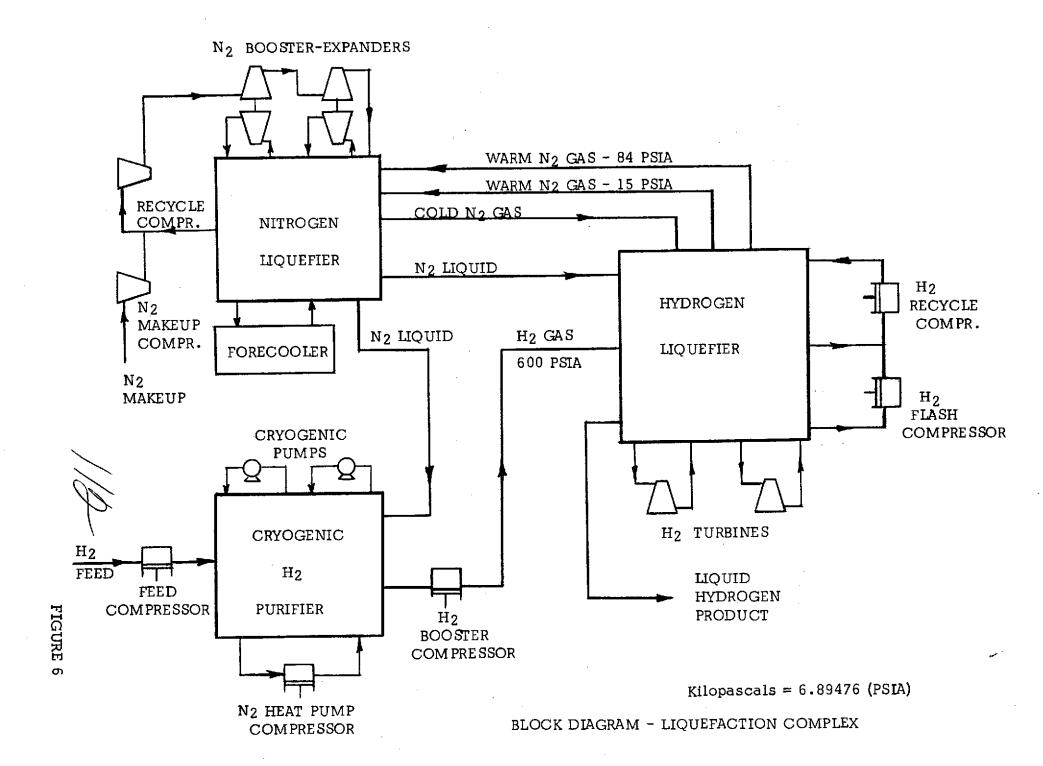
MINIMUM THEORETICAL WORK FOR

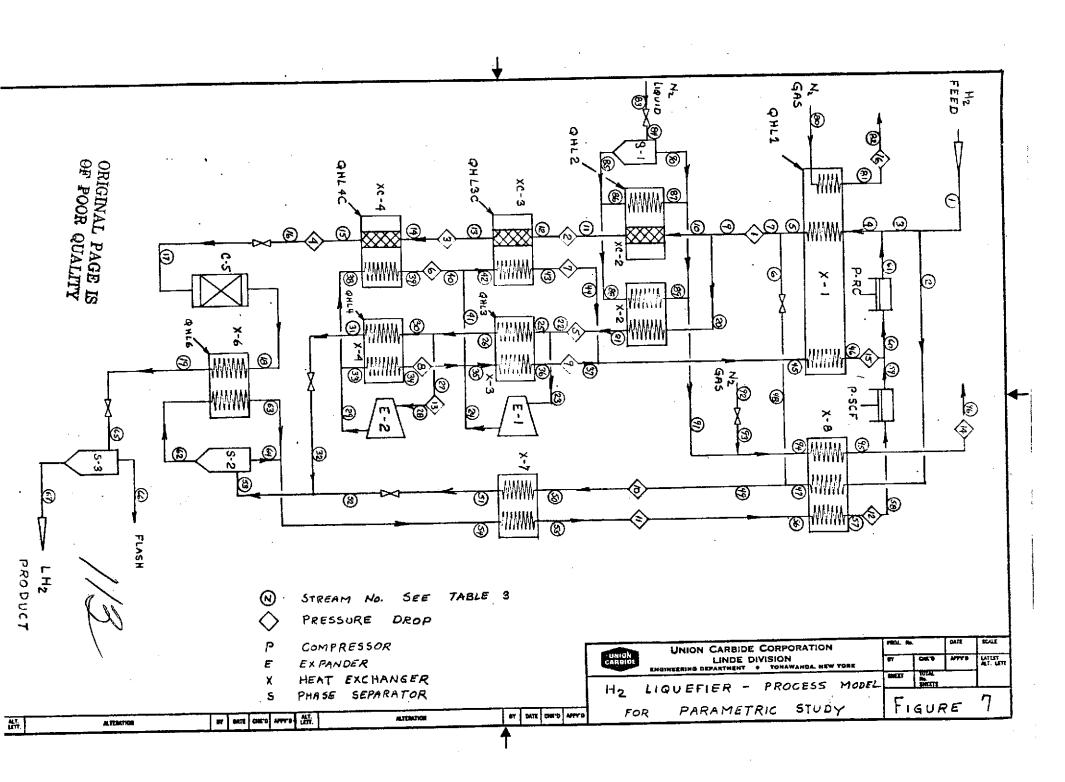
LIQUEFACTION OF H2

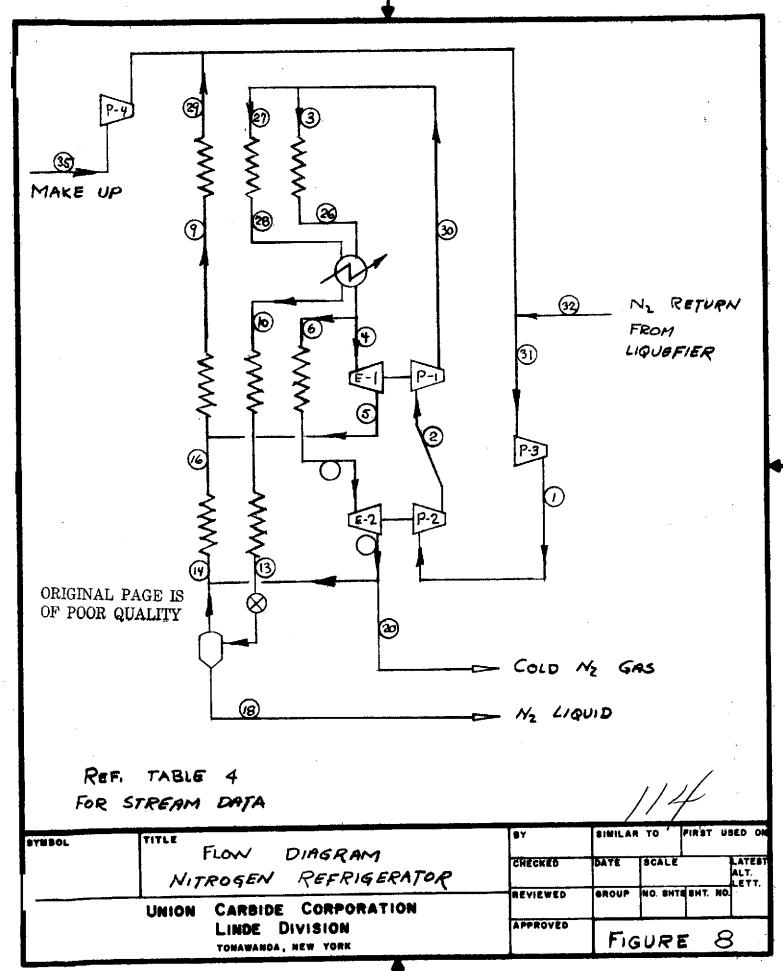
٧S

PARA H2 CONTENT







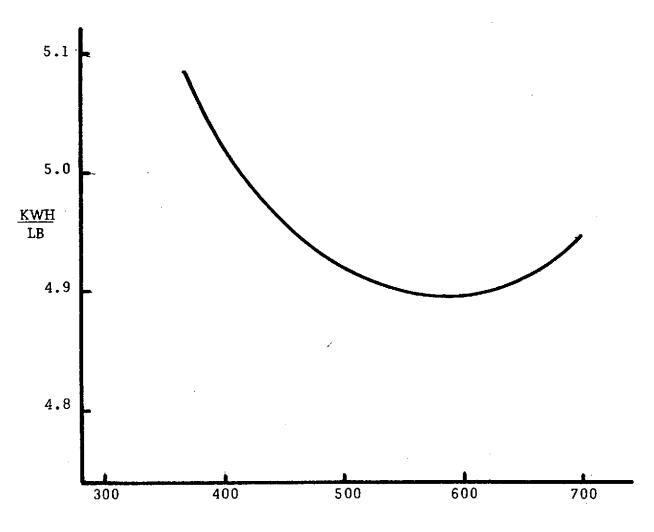


ACTUAL WORK FOR

LIQUEFACTION OF H2

VS

H2 LIQUEFIER FEED PRESSURE



FEED PRESSURE - PSIA

115

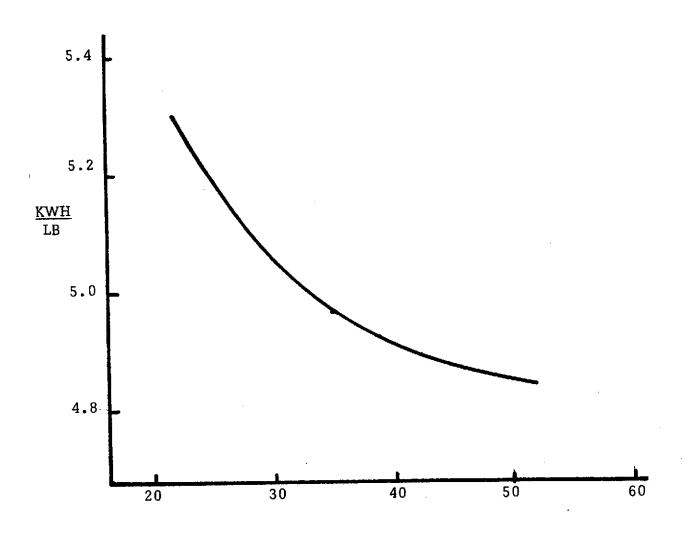
FIGURE 9

Kilojoules/gm = 7.9367 (KWH/LB)
Kilopascals = 6.89476 (PSIA)

ACTUAL WORK FOR
LIQUEFACTION OF H₂

VS

H₂ RECYCLE PRESSURE



Kilojoules/gm = 7.9367 (KWH/LB)

Kilopascals = 6.89476 (PSIA)

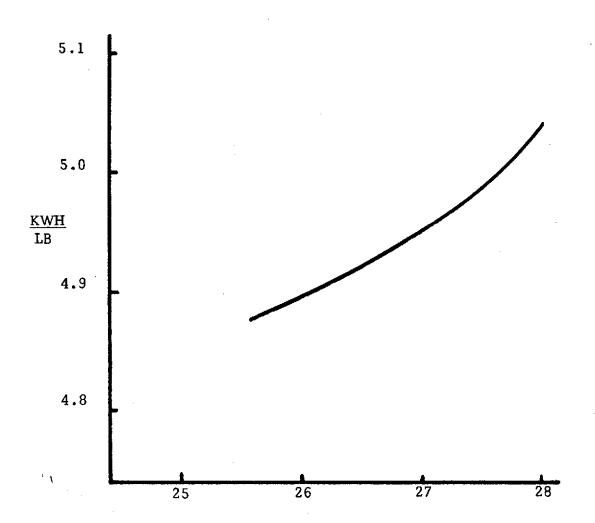
RECYCLE PRESSURE - PSIA

ACTUAL WORK FOR

LIQUEFACTION OF H2

٧S

MINIMUM REFRIGERATION LEVEL

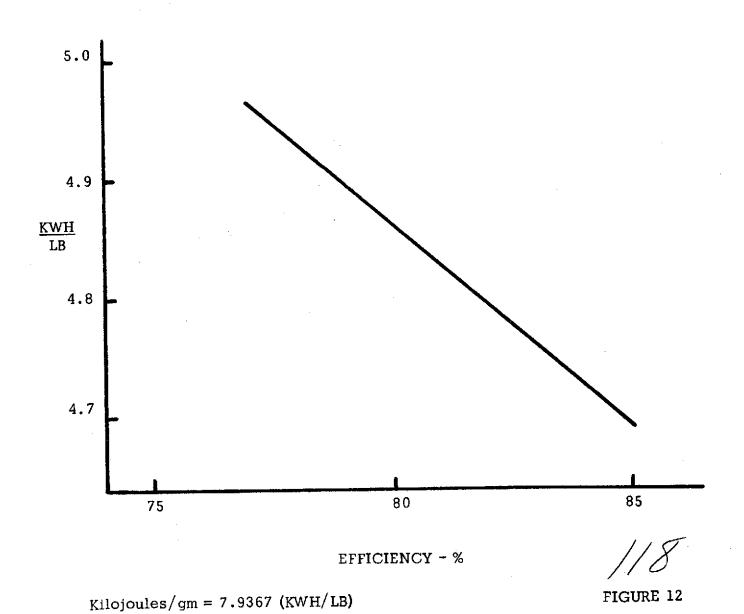


REFRIGERATION LEVEL - °K

FIGURE 11

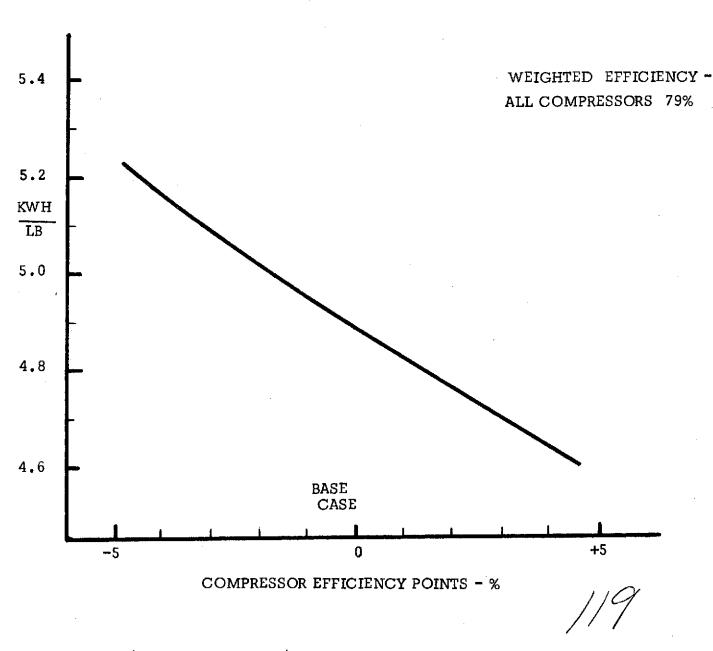
Kilojoules/gm = 7.9367 (KWH/LB)

ACTUAL WORK FOR
LIQUEFACTION OF H₂
VS
H₂ TURBINE EFFICIENCY



ACTUAL WORK FOR LIQUEFACTION OF $\rm\,H_2$

'S
COMPRESSOR EFFICIENCY

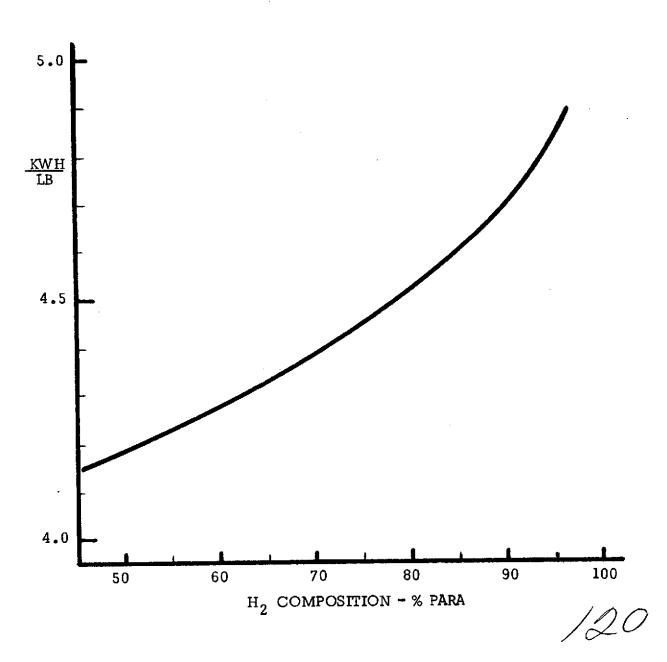


Kilojoules/gm = 7.9367 (KWH/LB)

FIGURE 13

ACTUAL WORK FOR LIQUEFACTION OF H₂

VS PARA CONTENT



Kilojoules/gm = 7.9367 (KWH/LB)

FIGURE 14

ACTUAL WORK FOR LIQUEFACTION OF $\rm H_2$

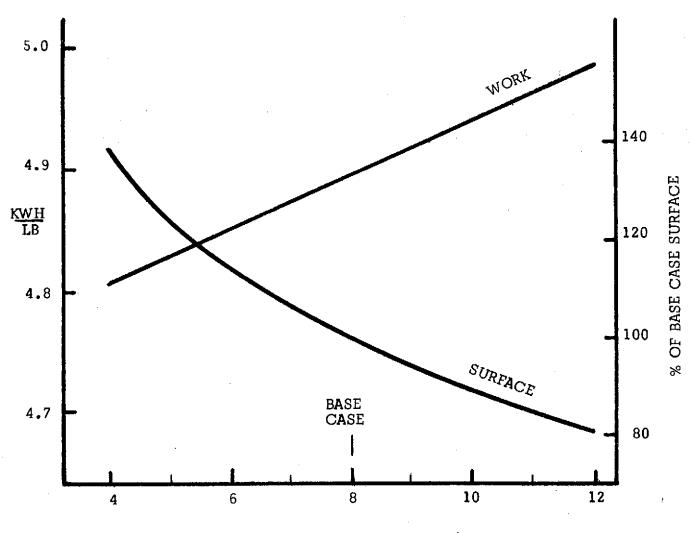
AND HEAT TRANSFER SURFACE

VS

WARM END TEMPERATURE APPROACH

FOR EXCHANGERS

X - 1 AND X - 8

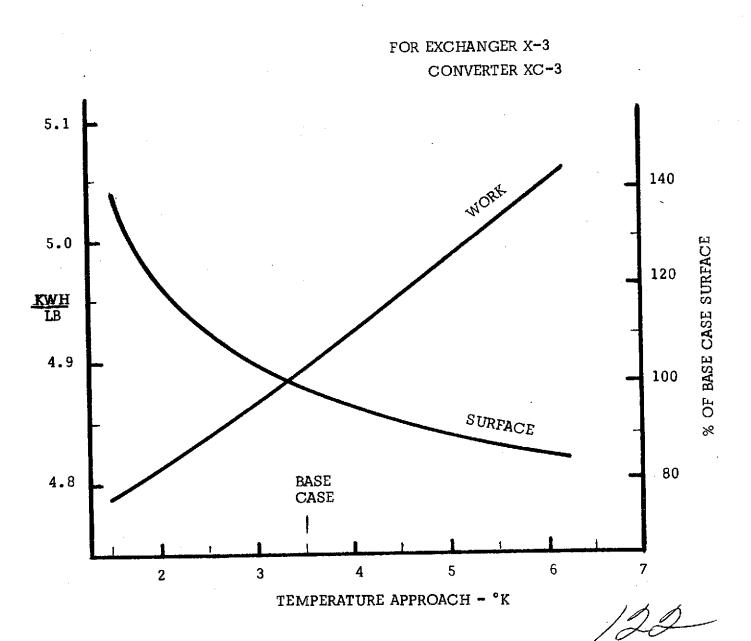


TEMPERATURE APPROACH - °K

FIGURE 15

Kilojoules/gm = 7.9367 (KWH/LB)

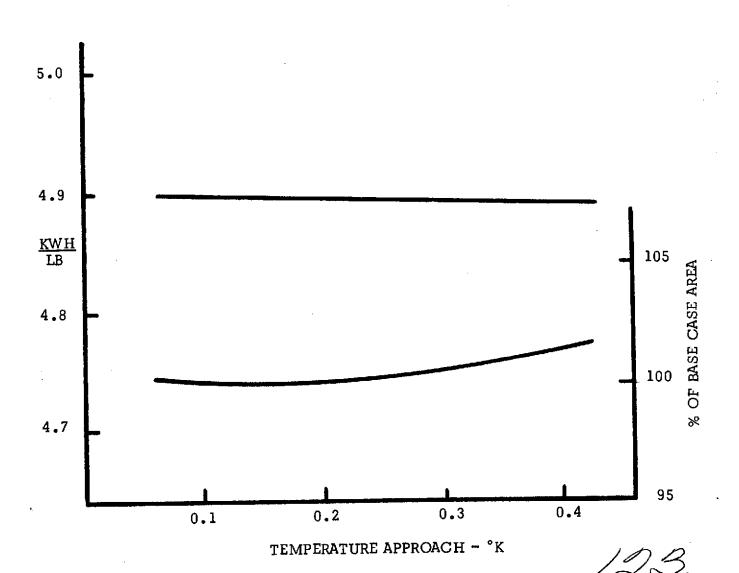
ACTUAL WORK FOR LIQUEFACTION OF H₂ AND HEAT TRANSFER SURFACE VS WARM END TEMPERATURE APPROACH



Kilojoules/gm = 7.9367 (KWH/LB)

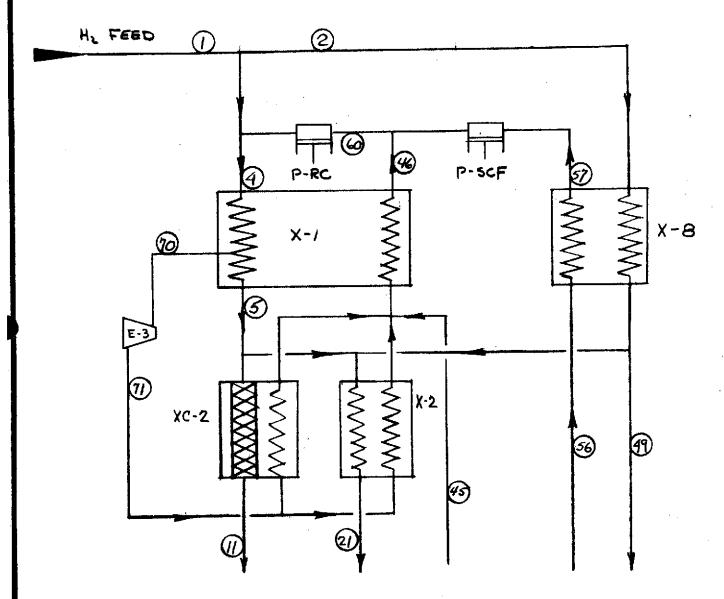
FIGURE 16

ACTUAL WORK FOR LIQUEFACTION OF H₂ AND HEAT TRANSFER SURFACE VS COLD END TEMPERATURE APPROACH FOR EXCHANGER X-2 CONVERTER XC-2



Kilojoules/gm = 7.9367 (KWH/LB)

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REF. TABLE 7 FOR
PROCESS CONDITIONS

SIMILAR TO FIRST USED ON CHECKED DATE SCALE LATEST ALT.
REVIEWED SROUP NO. SHTS SHT. NO.

UNION CARBIDE CORPORATION LINDE DIVISION

TONAWANDA, NEW YORK

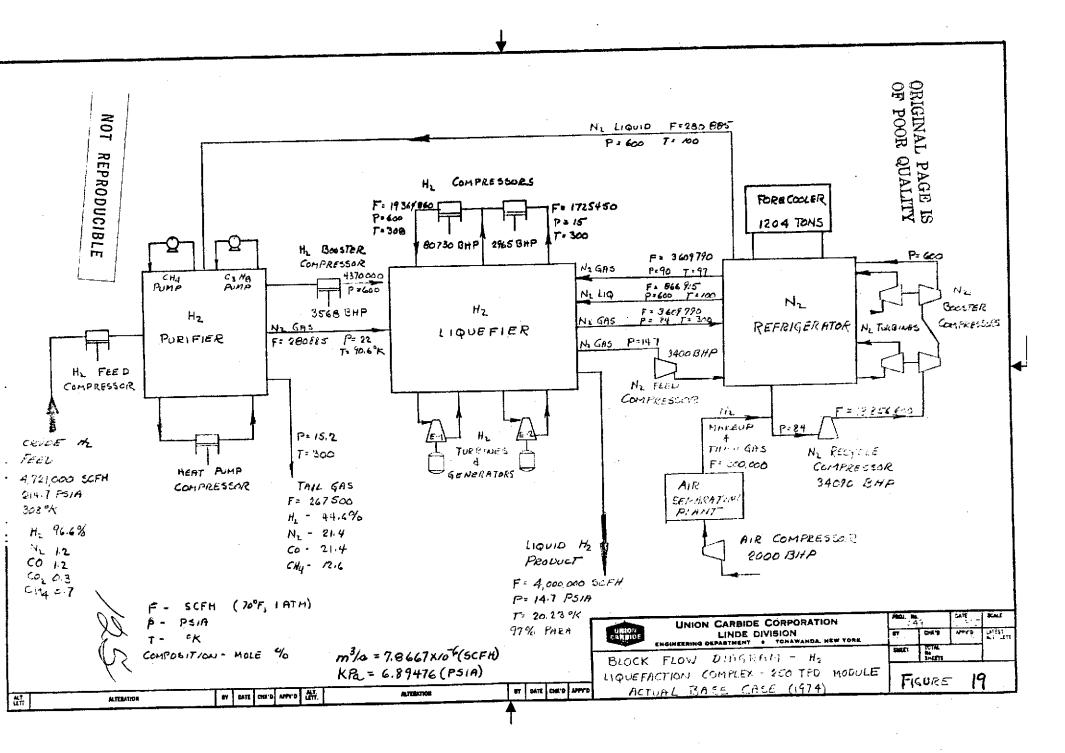
ALTERNATE REFRIGERATION -

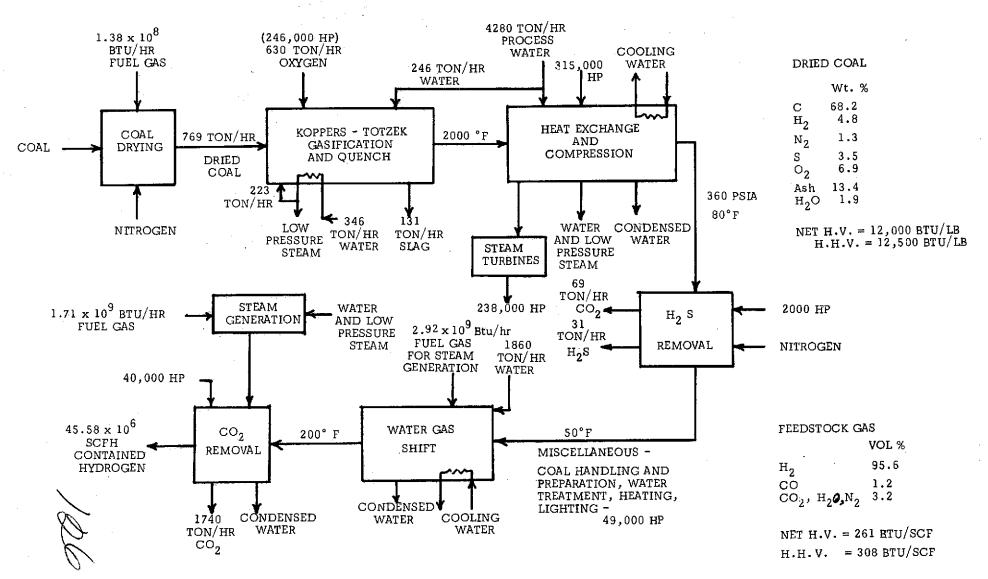
PRECOOLING VIA H2 EXPANSION

APPROVED

FIGURE 18

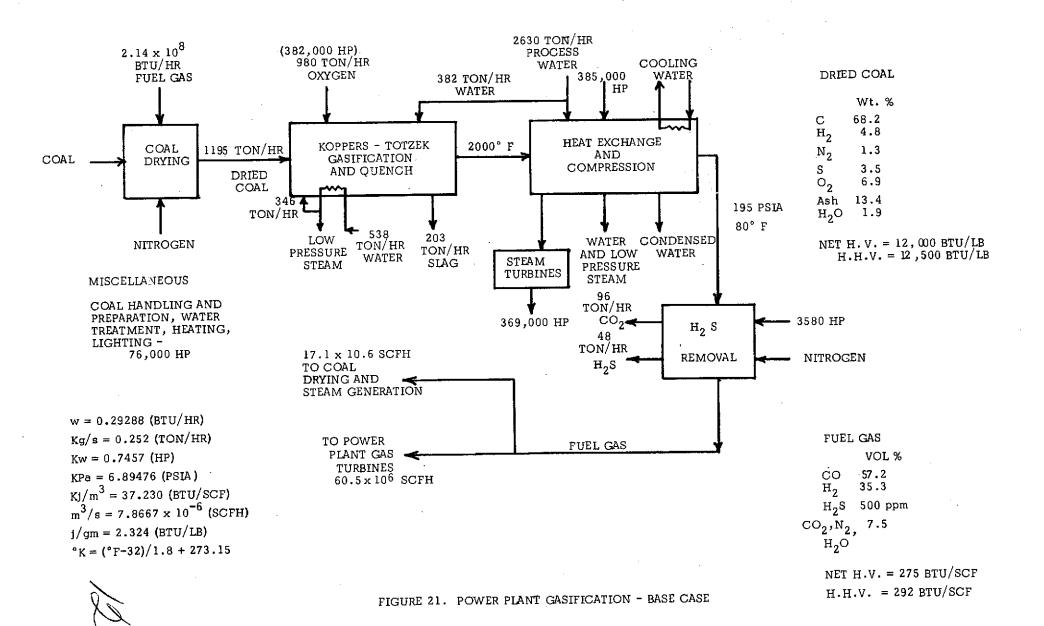
SYMBOL

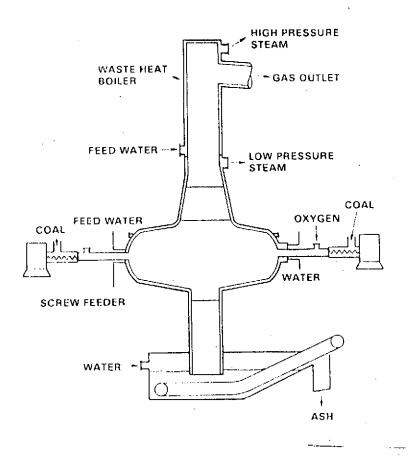




REFER TO FIGURE 21 FOR CONVERSION FACTORS

FIGURE 20. FEEDSTOCK GASIFICATION - BASE CASE



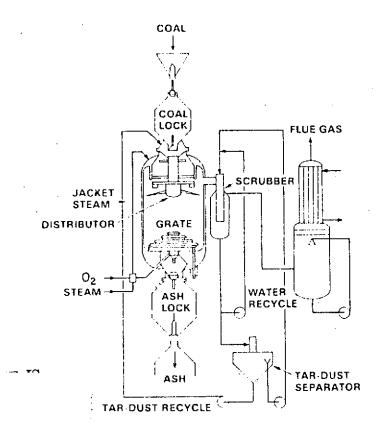


Koppers-Totzek

TYPICAL RAW GAS COMPOSITION

Component	Mole %
СО	50.4
CO2	5.6
H ₂	33.1
H₂O	9.6
CH ₄	0.0
H ₂ S+COS	0.3
N_2	1.0
Total	100.0

Higher Heating Value (dry basis) 298 Btu/Scf



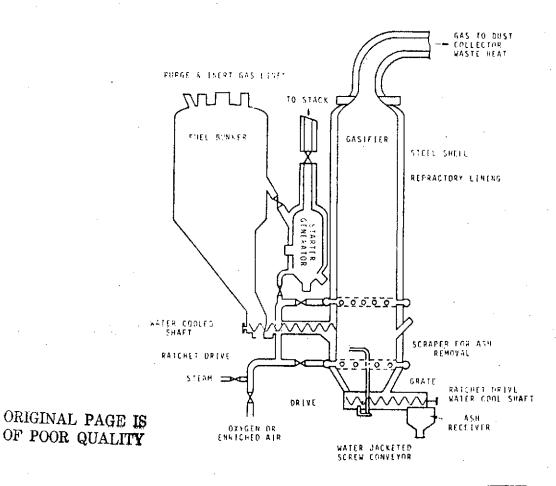
Lurgi Gasification

TYPICAL RAW GAS COMPOSITION

Component	mol %
СО	9.2
CO ₂	14.7
H_2	20.1
H ₂ O	50, 2
CH₄	4, 7
C_2H_6	0, 5
Other and H ₂ S	0.6
Total	100.0
Higher Heating Value (Dry Basis)	302 Btu/SCF

Kilojoules/ $m^3 = 37.23$ (Btu/SCF)

129



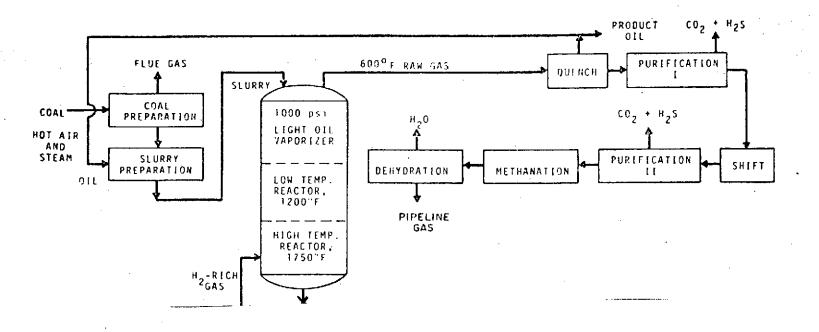
Winkler Process

TYPICAL RAW GAS COMPOSITION (For coal having sulfur less than 1%)

Component	mol %
со	25.7
CO2	15.8
H_2	32, 2
H₂O	23.1
CH ₄	2.4
N ₂	0.8
H₂S	· 2500 ppm
cos	400 ppm //
Total	100.00
Higher Heating Valu	ne (Dry Basis) 275 Btu/SCF

Kilojoules/ $m^3 = 37.23$ (Btu/SCF)

HYGAS



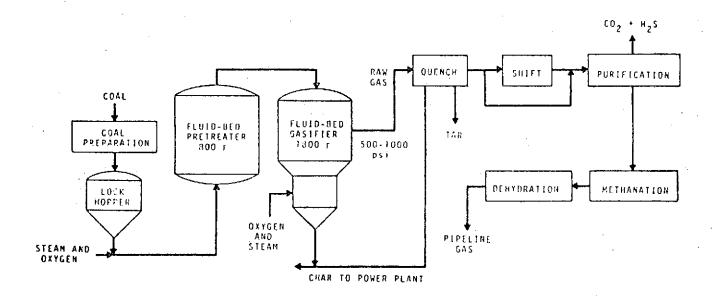
TYPICAL RAW GAS COMPOSITIONS

<u></u>	Electrothermal	Oxygen Gasifier	Steam-Iron
Component		mol %	
со	21.3	18.0	7.4
CO2	14.4	18,5	7. 1
H ₂	24,2	22,8	22,5
H₂O	17.1	24.4	32, 9
CH₄	19.9	14.1	26, 2
C₂H₄	0.8	0, 5	1.0
H ₂ S	1, 3	0,9	1.5
Other	1,0	0.8	1.4
Total	100.0	100,0	100.0
Higher Heating Value (Dry Bas	437 Btu/SCF	374 Btu/SCF	565 Btu/SCF

 $Kilojoules/m^3 = 37.23 (Btu/SCF)$

 $^{\circ}K = (^{\circ}F-32)/1.8 + 273.15$

Kilopascals = 6.89476 (PSIA)



SYNTHANE Process

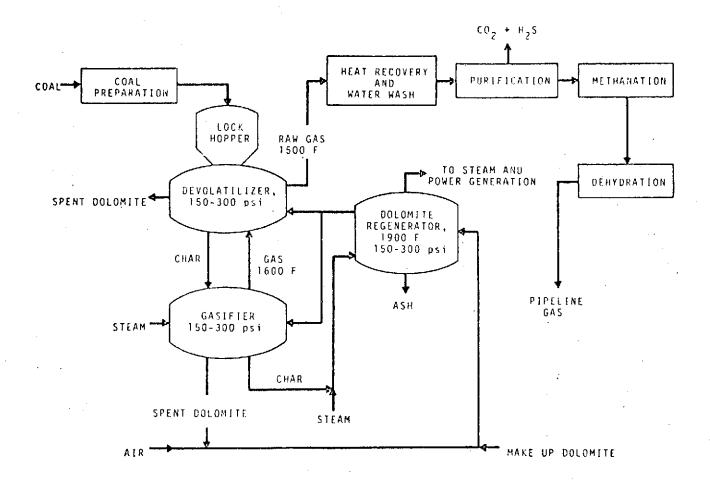
TYPICAL RAW GAS COMPOSITION

·	
Component	mol_%
СО	10, 5
CO2	18.2
H_2	17.5
H ₂ O	37.1
CH₄	15.4
C ₂ H ₆	0,5
H ₂ S	0, 3
N ₂	0, 5
Total	100.0
Heating Value (Dry Basis)	405 Btu/SCF

Higher H

Kilojoules/m³ = 37.23 (Btu/SCF) $^{\circ}K = (^{\circ}F-32)/1.8 + 273.15$ Kilopascals = 6.89476 (PSIA)

FIGURE 26

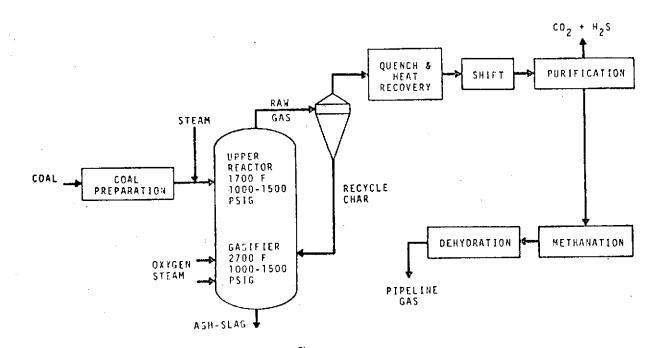


CO2-ACCEPTOR PROCESS

TYPICAL RAW GAS COMPOSITION

	TYPICAL	KAW GAS	COMPOSITION	*	
Con	mponent		mo	01 %	
С	0		14	4.1	•
. C	O _z		!	5, 5	
Н	2		44	4.6	
Н	_z O		1	7. 1	
С	H_4		1	7.3	
C	zH ₆			0.37	
N	I ₂		1	0,2	
N	IH ₃			0.8	
·	I ₂ S			0.03	Inh
	Total		10	0.00	135
F	ligher Heating	Value (Dry E	Basis)	440 Btu/CF	•

Kilojoules/m³ = 37.23 (Btu/CF) °K (°F-32)/1.8 + 273.15 Kilopascals = 6.89476 (PSIA)



BIGAS PROCESS

TYPICAL RAW GAS COMPOSITION

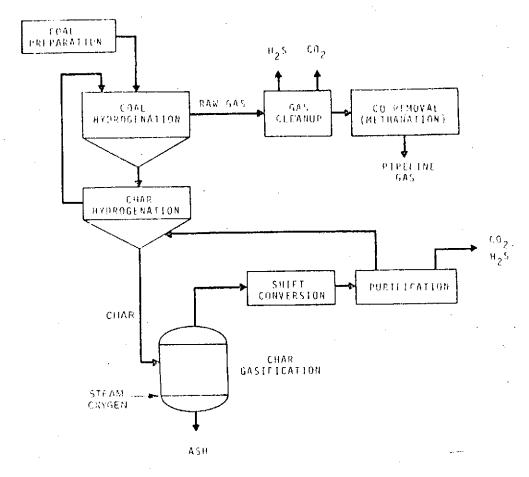
Component_	mol %
CO	22,9
CO2	7.3
H_2	12.7
H₂O	48.0
CH ₄	8.1
H₂S	0.7
N _Z	0.3
Total	100,0
ting Value (Dry Basis)	378 Btu/SCF

Higher Heat

Kilojoules/ $m^3 = 37.23$ (Btu/SCF)

 $^{\circ}K = (^{\circ}F-32)/1.8 + 273.15$

Kilopascals = 6.89476 (PSIA)



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HYDRANE PROCESS

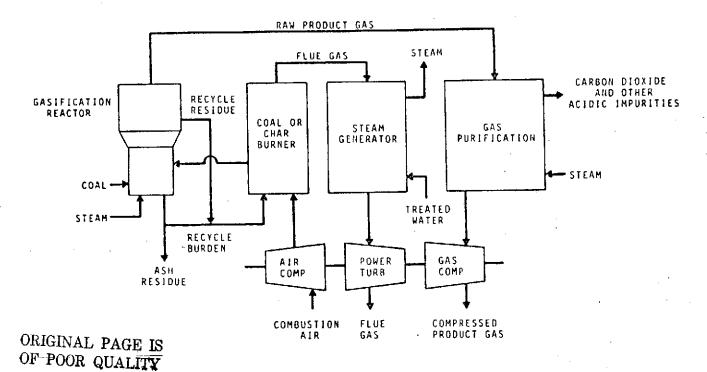
TYPICAL RAW GAS COMPOSITION

Component		Mol %
CH₄		73.2
H ₂		22.9
co		3.9
	Total	100.0

Higher Heating Value (Dry Basis) 826 Btu/SCF

Kilojoules/ $m^3 = 37.23$ (Btu/SCF)

135



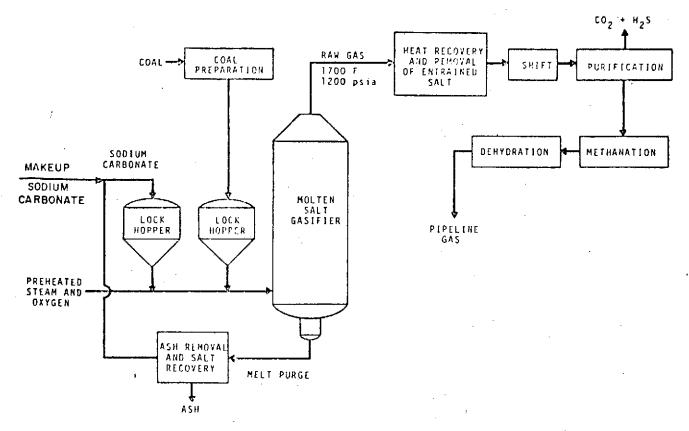
UNION CARBIDES! AGGLOMERATED-ASH PROCESS

Gasifier Raw Product Gas

Raw product gas from the gasifier of approximately the following composition:

Pressure	100-150 psig	150-300 psig
Temperature	1,900°F	1,750°F
Methane	2%	12%
Hydrogen	50%	33%
Carbon Monoxide	25%	18%
Carbon Dioxide	5%	0.65%
Hydrogen Sulfide	0.45%	0.45%
Carbonyl Sulfide	0.05%	0.05%
Water	18.0%	26.0%
Ammonia	0.6%	0.70%

 $^{\circ}K = (^{\circ}F-32)/1.8 + 273.15$ Kilopascals = 6.89476 (PSIG + 14.7)



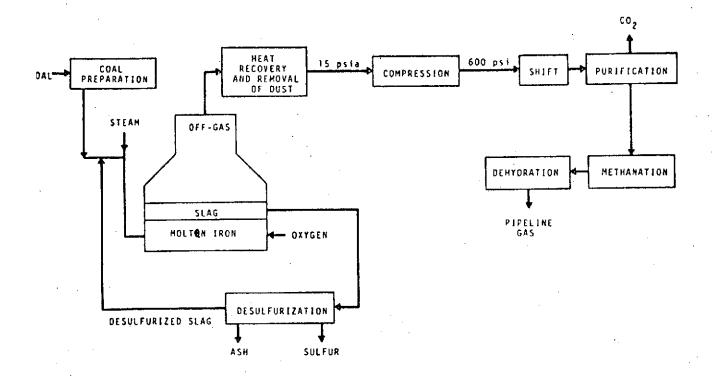
KELLOGG MOLTEN-SALT PROCESS

TYPICAL RAW GAS COMPOSITION

Component	Mole %
СО	26.0
CO	10.3
CH_4	5.8
H ₂	34.8
H ₂ S	0.2
N_2	0.3
H₂O	22.6
	100.0

Higher Heating Value (dry basis) 329 Btu/SCF

Kilojoules/m³ = 37.23 (Btu/SCF) Kilopascals = 6.89476 (Psia) $^{\circ}$ K = ($^{\circ}$ F-32) /1.8 + 273.15



ATGAS Process

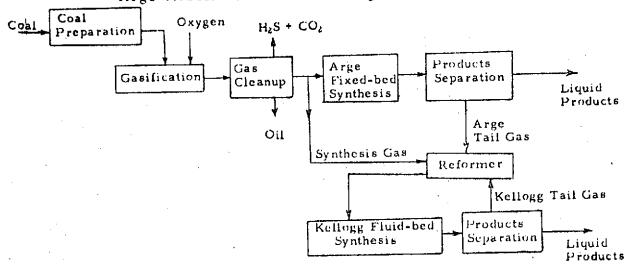
Kilopascals = 6.89476 (Psia)

TYPICAL RAW GAS COMPOSITION

Component	mol %
СО	69.7
H_2	9.6
CH₄	20,0
N_2	0,7
Total	100.0
Higher Heating Value (Dry Basis)	457 Btu/SCF
	138
Kilojoules/ $m^3 = 37.23$ (Btu/SCF)	FIGURE 32

FISCHER-TROPSCH SYNTHESIS

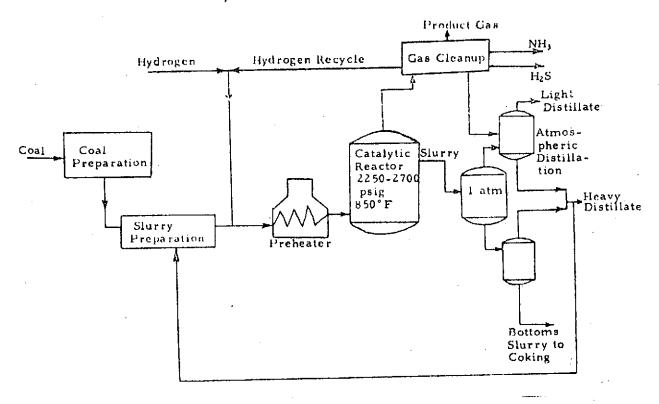
M. W. Kellogg Co. and Arge-Arbeit Gemeinschaft Lurgi and Ruhrchemie



Typical Products	Fixed Bed Process Liquid Produc	Fluid Bed Process t Composition—
Liquified Petroleum Gas (C3 - C4)	5,6	7.7
Petrol (C5 - C11)	33,4	72.3
Middle Oils (diesel, furnace, etc.	16.6	3.4
Waxy Oil or Gatsch	10.3	3.0
Medium Wan, mp 135-140°F	11.8	
Hard Wax, mp 203-206°F	18.0	
Alcohols and Ketones	4.3	12,6
Organic Acids	traces	1.0

	Fixed Bed Process		Fixed Bed Process	
		Liquid Product		
	C5-C10	C 11- C 18	C5-C10	C11-C14
Paralins, Vol %	45	55	13	15
Olefins	50	40	70	60
Aromatics	0	0	5	15
Alcohols	5	.5	6	5
Carbonyls	traces	traces	6	.5
		•		129
$c = (^{\circ}F-32)/1.8 + 2$	73.15			FIGURE 33

H-COAL Hydrocarbon Research, Inc.



Typical Products

Typical products from Illinois No. 6 Bituminous coal are as follows:

IBP Cuts	Volume %	Gravity CAPI
IBP - 400°F	42.18	44.6
400-650°F	41,51	17.3
650-975°F	16.31	5.0
	100.00	25. 2

Kilopascals = 6.89476 (psig + 14.7)

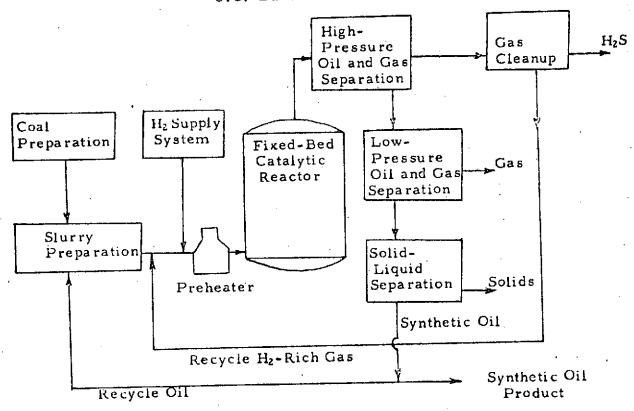
Kilopascals = 101.325 (atm)

 $^{\circ}K = (^{\circ}F-32)/1.8 + 273.15$

140

SYNTHOIL

U.S. Bureau of Mines



Hydrodesulfurization of Kentucky Coal.

Experimental Conditions:	
Liquid Feed Throughput: 140 lb./hr./ft. Reactor Volum Slurry Feed: 45 Ccal/55 Recycle Oil Hydrogen Recycle Rate: 125 std. cu. ft./hr. Pressure: 4,000 lb./sq. in. gauge	ne
Temperature: 450°C	
Sulfur in Feed Coal, wt. %	. 4.6 . 0.19
Sulfur in Recycle Oil (Product Oil), wt. %	•
Solvent Analysis of Product Oil, wt. % Oil (Pentane Soluble)	, 79.5
Asphaltene	. 11.7
Organic benzene insolubles	. 2.1
Ach	, 1.0
Elemental Analysis of Product Oil (Ash-Free), wt. %	
Carbon	. 89.9
Hydrogen	. 9.2
Nidwagan	. 0.17
via and its of Product Oil SSF at 180°F	. 21-30
Calorific Value of Product Oil, B.t. u. /lb	-/4/-
NOT REPRODUCIBLE	FIGURE 35

FIGURE 35 (CONT'D.)

```
gm/s, m^3 = 4.4491 (lb/hr/ft<sup>3</sup>)

m^3/s = 7.8667 \times 10^{-6} (std. cu. ft./hr.)

Kilopascals = 6.89476 (lb/sq. in. gauge + 14.7)

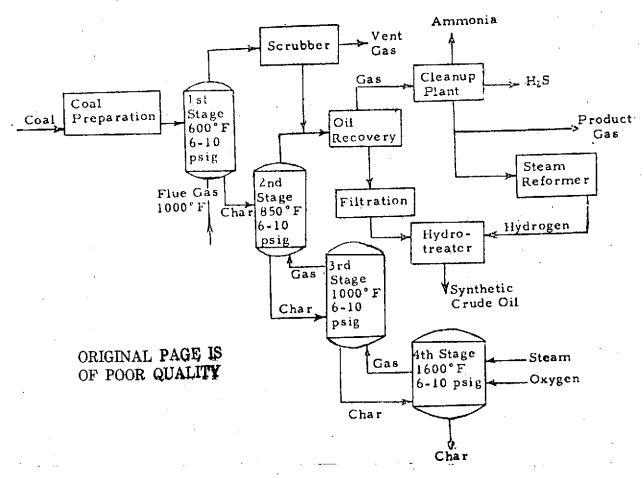
°K = °C + 273.15

Joules/gm = 2.3244 (Btu/lb)
```

-/40-

COED PROCESS

FMC Corporation



Typical Products

Some yield data for pyrolysis of Illinois No. 6 seam coal.

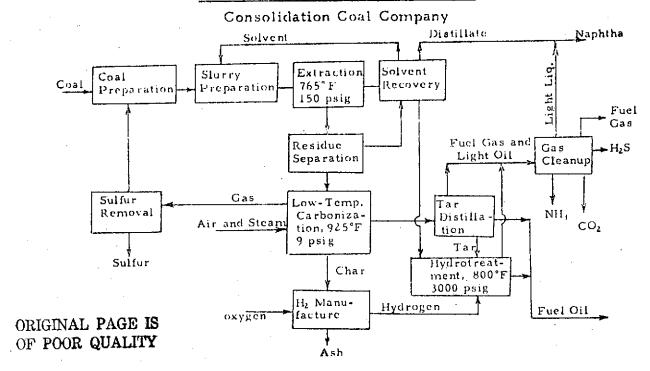
a.	Net Process Yield	Pyrolysis Weight % of Dry Coal
Char	1177 lb/ton	59. 1
Oil	1.04 bbl/ton	19. 6
Liquor	7.1 Gal/ton	5.5
Gas	8133 SCF/ton	15.8
Total		100.0

gm/Kg = 0.500 (lb/ton) $m^3/Kg = 1.7525 \times 10^{-4} \text{ (bbl/ton)}$ $m^3/Kg = 4.1727 \times 10^{-6} \text{ (Gal/ton)}$ $m^3/Kg = 3.1217 \times 10^{-5} \text{ (SCF/ton)}$ Kilopascals = 6.89476 (psig + 14.7)K = (F-32)/1.8 + 273.15

143

FIGURE 36

CONSOL SYNTHETIC FUEL (CSF)



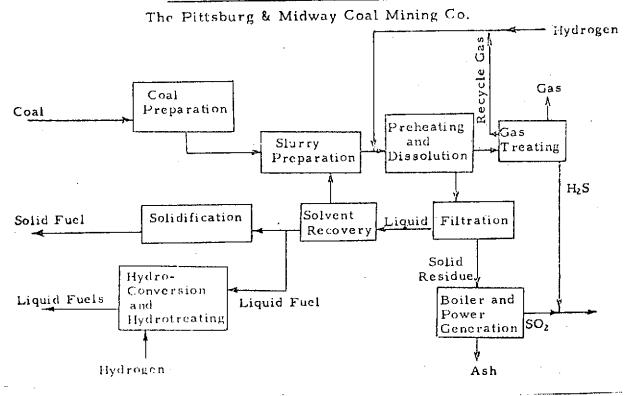
TYPICAL PRODUCTS USING PITTSBURGH SEAM COAL (IRELAND MINE)

Product	Product/Ton o	of Raw Coal	Characteristics of Products
Gas	3, 424	MSCF	HHV 933 Btu/SCF
Naphtha	0.52	bbl	58 OAPI, 5.2 MMBtu/bbl,0.056 Wt%S
Fuel Oil	1.52	b b1	10.3°API, 6.3 MMBtu/bbl,0.128 Wt%S
Ammonia	11.00	1b .	
Sulfur	71.00	1b	
Ash	213.60	1b	•

$$m^3/Kg = 0.031217 \text{ (MSCF/TON)}$$

 $m^3/Kg = 1.7525 \times 10^{-4} \text{ (bbl/ton)}$
 $gm/Kg = 0.500 \text{ (lb/ton)}$
 $Kilojoules/m^3 = 37.23 \text{ (Btu/SCF)}$
 $Kilojoules/m^3 = 6.632 \times 10^6 \text{ (MM Btu/bbl)}$
 $Kilopascals = 6.89476 \text{ (psig + 14.7)}$
 ${}^{\circ}K = ({}^{\circ}F-32)/1.8 + 273.15$

SOLVENT REFINED COAL (SRC)

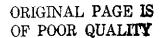


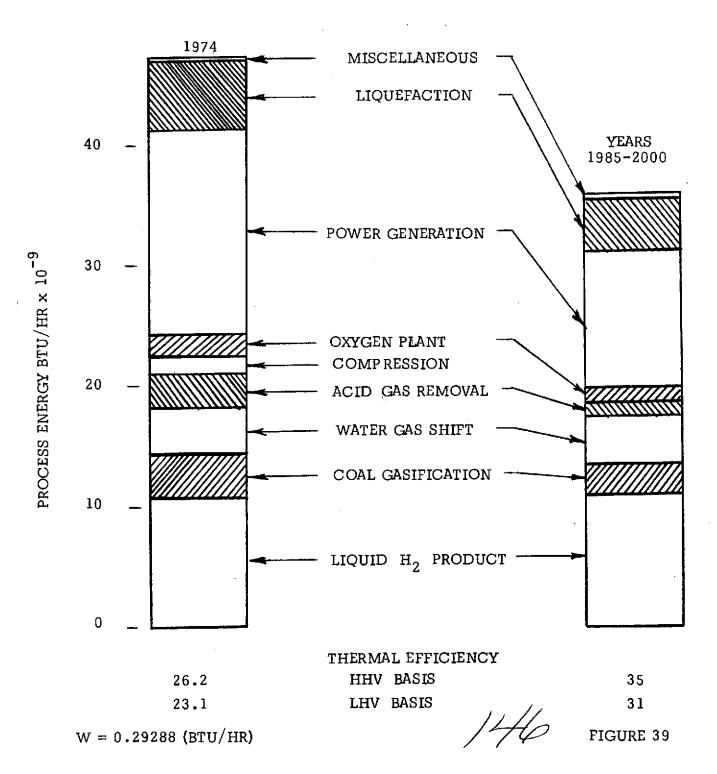
Typical Products	Raw Coal	Product Solvent Refined Coal
Carbon	70.7 Wt. %	88.2
Hydrogen	4.7	5, 2
Nitrogen	1, 1	1.5
Sulfur	3, 4	1.2
Oxygen	10.3	3.4
Авh	7, 1	0.5
Moisture	2.7	100.0
Volatile matter	38,7	36.5
Fixed Carbon	51,5	63.0
Ash	7, 1	0.5
Moisture	2,7	
•	100.0	100.0
Btu/lb	12,821	15,768

Joules/gm = 2.3244(Btu/lb)

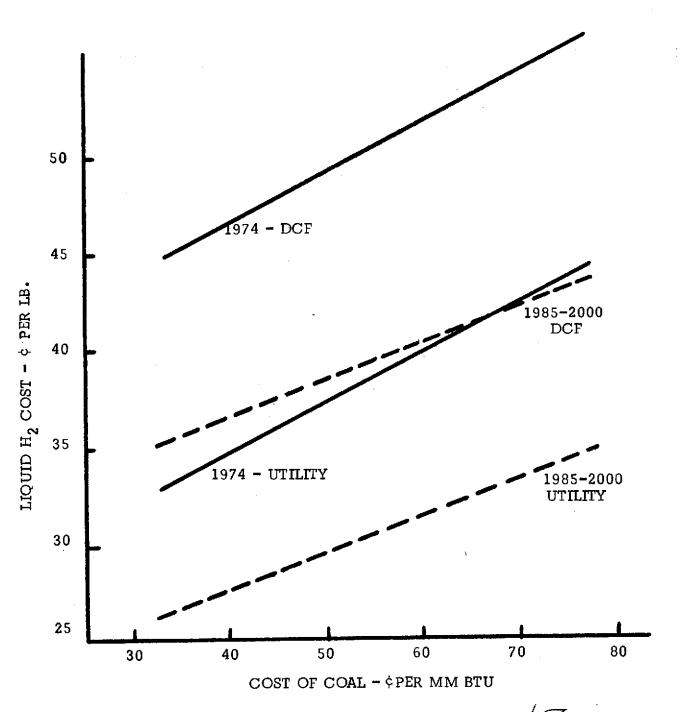
DISTRIBUTION OF PROCESS

ENERGY PRESENT AND FUTURE



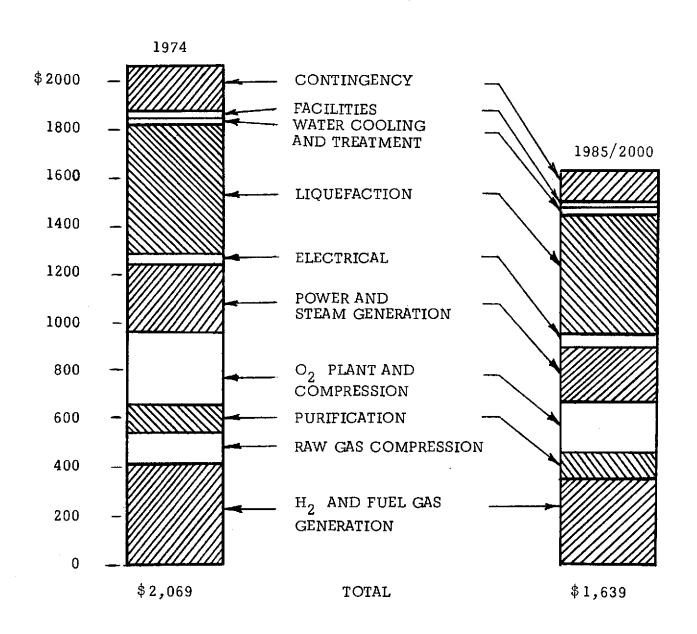


TOTAL UNIT COST OF LIQUID H₂ VIA COAL GASIFICATION



¢ kilojoule = 9.4845×10^{-7} (¢ per MM BTU) ¢ Kg = 2.2046 (¢/lb) /// FIGURI

SUMMARY OF TOTAL PLANT INVESTMENT PRESENT AND FUTURE (MILLIONS OF DOLLARS)



///8 FIGURE 41